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Stopping Power of Fast Charged Particles in Heavy Elements

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The stopping power formula from Bethe's theory contains terms which are known only approximately and must be estimated with the use of experimental data. These terms include a material constant, the mean excitation energy of the medium, and the shell-, Bloch- and Barkas-corrections. In an analysis of measured proton and alpha-particle stopping powers and ranges, modifying parameters have been introduced into these corrections, and the mean excitation energy was simultaneously adjusted, so as to get the closest possible agreement with experimental results. Such an analysis is reported here for elements with atomic numbers $Z \geq 57$. The modification parameters introduced for the shell corrections have a simple relation to atomic energy levels. The Bethe theory with the adopted mean excitation energies and proposed adjustments of the shell- and Barkas-corrections predicts stopping powers that are in close agreement with experimental values, within the experimental uncertainties. This agreement was obtained for protons with kinetic energies above about 0.5 MeV, and for heavier ions of charge z at energies above $(z - 1.5)$ MeV/u.

Report of work done under contract for the National Institute of Standards and Technology

I. INTRODUCTION

The Bethe-Bloch theory of stopping power, S , (Bethe, 1930; Bloch, 1933; Fano, 1963) with a Barkas effect correction term and including shell corrections has been shown to agree well with experimental data for protons and alpha particles with kinetic energies T/M (M is the number of nucleons in the particle) above 0.5 MeV traversing light elements for which I -values had been determined independently. A single free parameter for the Barkas effect was introduced (Bichsel and Porter, 1982). For heavier elements, semiempirical I -values and shell corrections were used to calculate S for comparison with experimental data (e.g. Bichsel, 1961; Bichsel, 1972; Janni, 1982; Porter and Bryan, 1984; ICRU, 1984). Since shell corrections for the M -shells (Bichsel, 1983) and the separate L -subshells (Bichsel, 1987) are now available, I have explored the validity of the theory with these functions. It was necessary to introduce corrections for the outer (N , O , P , Q) shells: they were derived from the M -shell corrections with a scaling procedure using atomic structure data. For all elements with $57 \leq Z \leq 92$, the I -value was the only free parameter not simply related to Z . The theoretical Bloch function L_2 and an empirical function L_1 for the Barkas effect (Bichsel, 1990) were used.

The present study is an outgrowth of earlier work (Bichsel, 1961, 1964, 1967) and is an effort complementary to those by Andersen and Ziegler (1977), Ziegler (1977) and Janni (1982). Many observations about problems with experimental data were made in these references and should be studied there.

II. THEORY

The theory of S for heavy elements is complex (see Table XI below). It is not possible to calculate S a priori with an accuracy of, say, 1%, and empirical modifications of the current a priori theoretical functions are needed to get calculated values S_t agreeing with experimental data S_x . These modifications are attained by varying the values of parameters in the functions. Many of the parameters are quite interdependent: a change in a parameter causing an increase

in S over an extended energy range can readily be compensated by a change in one of the other parameters causing a decrease in S (see Table IV below).

It is the purpose of the present paper to consider the complete theory of S outlined below, and parameters used should have values plausibly related to atomic data. In other analyses, incomplete theories (e.g. Janni, 1982, did not explicitly use z^3 and z^4 corrections) or polynomial fits to the shell corrections (where the parameters have no physical significance) were used (Andersen and Ziegler, 1977). The same goal is achieved with all these approaches: semiempirical functions are given which approximate the experimental data.

Further improvements in the theory of interactions of charged particles with matter have been achieved for collision cross sections (e.g. Anholt, 1979, Cohen and Harrigan, 1985), but similar improvements have not been made for the stopping power. Relativistic corrections for atomic properties are discussed in the Appendix, but were not used in the data analysis

A. Stopping power, S.

The expression used for the calculation of the stopping power of fast charged particles is

$$S = - \frac{dT}{dx} = \frac{k}{\beta^2} \frac{Z}{A} z^2 L \quad [1]$$

with T the kinetic energy (MeV) of the particle,
 x the absorber thickness, g/cm²,
 $k = 4\pi e^4 N_0 / mc^2 = 4\pi r_0^2 N_0 mc^2 = 0.307072 \text{ MeV cm}^2$,
 $v = \beta c$ the speed of the incident particle,
 $\gamma^2 = 1/(1-\beta^2)$, $\gamma = 1 + T/M_0 c^2$,
 ze the charge of the incident particle,
 e the electron charge,
 m the electron rest-mass, $mc^2 = 511,000 \text{ eV}$,
 c the speed of light,
 $r_0 = 2.817941 \cdot 10^{-13} \text{ cm}$ the classical electron radius,
 $N_0 = 6.022045 \cdot 10^{23} \text{ atoms/mole}$, Avogadro's number,

Z the atomic number of the absorber,
 A the atomic weight of the absorber (in g),
 L the stopping number (B in older papers), and
 M_0 the rest mass of the particle; $p: M_0 c^2 = 938.2561 \text{ MeV}$
 $\alpha: M_0 c^2 = 3727.316 \text{ MeV}$
 Either β or T will be used as the variable indicating the particle energy, with $\beta^2 = (T/M_0 c^2) \cdot (2 + T/M_0 c^2) / (1 + T/M_0 c^2)^2$.

For particles heavier than electrons, the stopping number L is expressed in the form

$$L(z) = L_0 + zL_1 + L_2(z) \quad [2]$$

with

$$L_0(\beta) = f(\beta) - \ln I - \frac{C(\beta)}{Z} + (G(z, \beta) - \delta(\beta))/2 \quad [2a]$$

where $f(\beta) = \ln(2mc^2 \beta^2 \gamma^2) - \beta^2$, I is the mean excitation energy of the absorber, $C(\beta)$ the total shell correction, $G(z, \beta)$ the Mott correction term, δ the correction for the density effect, L_1 the Barkas correction term and L_2 the Bloch correction term. It is useful to define the experimental value of the stopping number, L_x , obtained by solving Eq. (1) for an experimental value S_x of the stopping power:

$$L_x(\beta) = S_x(\beta) \cdot A\beta^2 / (kz^2Z). \quad [2b]$$

B. I-values.

The mean excitation energy I is defined by

$$\ln I = \frac{\int_0^\infty f(E, 0) \ln E \, dE}{\int_0^\infty f(E, 0) \, dE}, \quad [3]$$

$$\int_0^\infty f(E, 0) \, dE = 1,$$

where E is the energy transfer in a transition and $f(E, 0)$ the dipole oscillator strength DOS (Fano, 1963), which is related to the optical absorption coefficient (e.g. Barkyoumb and Smith, 1990). The Bloch parameter is defined by

$$b \equiv I/Z$$

[3a]

For the Thomas-Fermi atom, Bloch (1933) showed that b is a constant.

For many gases, I -values have been determined with Eq. (3) (see, e.g., Zeiss et al., 1977; Jhanwar et al., 1983). The only metals for which I was calculated with Eq. (3) are Al (Shiles et al. 1980) and, partially, Si (Bichsel, 1988). For heavy elements, insufficient information is available about $f(E,0)$ to permit a determination of I .

For metals, the excitation function for the collective excitation of the valence electrons should be used in Eq. (3) ("plasmon excitations", e.g. Raether, 1980). Qualitatively, the influence of plasmons may be understood from the value of the most probable energy loss hf_v for valence electrons, given in Table VI; hf_v was derived from electron energy-loss spectra given by Ahn et al. (1983). hf_v depends on the structure of the metal and the number of valence electrons and thus will not relate simply to Z .

A quantity related to I is the plasma energy hf (Fano, 1963), defined by $(hf)^2 = 830.4 \rho Z/A$ (hf in eV, ρ the density of the metal in g/cm^3), shown in Table I. This quantity replaces the I -value in S for very high particle energies. Clearly, hf depends strongly on the density, explaining the small values for Pb, Bi and Th. The small values of hf_v and hf for Pb compared to those for Au may explain in part why the experimental value of the Bloch parameter, b_e , for Pb is smaller than that for Au.

Another approach to getting information about stopping power, I -values and shell corrections is to use the statistical atomic model (Bonderup, 1967). Values of I for atoms were calculated by Bichsel and Laulainen (1971) with this model using the relativistic wavefunctions of Liberman et al. (1965, 1971). The resulting Bloch parameters, b_L , based on $\gamma=1.347$, are given in Table I. Similar results were obtained by Chu and Powers (1972). Values for the solids would differ by several percent; for light elements there are large differences: for Al, $b(\text{atom})=9.56$ eV, Dehmer et al. (1975); $b(\text{solid})=12.77$ eV, Shiles et al. (1980); for Si,

$b(\text{atom})=9.39$ eV, $b(\text{solid})=12.43$ eV, Bichsel (1988). It must also be clearly understood that the DOS used in this model differs strongly from actual optical data (Johnson and Inokuti, 1983).

It is tempting to try to derive I-values from the well known experimental ionization energies J_1 (e.g. Bearden and Burr, 1967). I have used an expression given by Sternheimer et al. (1984) ((their Eq. (8)); it was derived for a different purpose) to calculate I from J_1 , the plasma frequency hf and with an estimate of DOS for photon energies above the ionization energies expressed by a factor τ . Values b_s calculated with a constant value $\tau=2$ are given in Table I. These results demonstrate that one should resist this particular temptation.

The experimental results for b_e from the present study are given in Table I, and are discussed in section III B. Experimental values used by Andersen and Ziegler (1977), Janni (1982) and ICRU (1984) are also given.

C. Shell corrections $C(v,Z)$.

1. General review.

In the Bethe theory, shell corrections must be calculated on a shell-by-shell basis:

$$C(v,Z) = \sum_{\nu} C_{\nu}(v,Z) = C_K(v,Z) + C_L(v,Z) + C_M(v,Z) + \dots \quad [4]$$

Usually, the dependence on particle speed v is expressed in terms of the variable η :

$$\eta_{\nu} = (mv^2/2) / (mv_0^2 \cdot Z_{\nu}^2/2) = (mv^2/2) / \epsilon_{\nu} \quad [4a]$$

with $\epsilon_{\nu} = RZ_{\nu}^2$, v_0 the Bohr speed ($v_0=c/137$), $R=mv_0^2/2 = 13.6$ eV the Rydberg energy of the hydrogen atom, and Z_{ν} the effective charge of the absorber atoms for electrons in shell ν . The dependence of C_{ν} on the atomic number Z also enters via the ionization energy J_{ν} , expressed in terms of:

$$W_{\nu} = J_{\nu} / \epsilon_{\nu}. \quad [4b]$$

In principle (Janni, 1982), these functions should be calculated for each subshell in the atom (Bearden and Burr, 1967). Here, a somewhat simpler approach was used, as outlined below.

Shell corrections for K- and L-shells were derived by Walske (1952, 1956) with the nonrelativistic hydrogenic approximation. Recently, the corrections for the M-shells (Bichsel, 1983) and the L-subshells have been calculated (Bichsel, 1987), also with the hydrogenic approximation.

For the outer shells no calculations have been made, and a scaling procedure was used in which it was assumed that the shell-corrections for outer shells have the same shape as those for the inner shells (Hirschfelder and Magee, 1948; Bichsel, 1961; Janni, 1982). Vertical, V_{ν} , and horizontal, H_{ν} , scaling factors were introduced:

$$C_{\nu} = V_{\nu} C_{\mu}(W_{\mu}, H_{\nu} \cdot \eta_{\mu}) \quad [5]$$

where ν stands for any one of the outer shells and μ stands for the inner shell. Presumably, H_{ν} would be proportional to the ratio of ionization energies, J_{μ}/J_{ν} , and V_{ν} related to the number of electrons in the shell. In order to assess the plausibility of this approach, it is instructive to compare the shapes of the known shell corrections. In Fig. 1, they are shown for K, L and M electrons in gold. The functions have been plotted in such a way as to coincide at the maximum value. Clearly, the functions are similar in shape, and the scaling procedure can be used with some justification, but the horizontal scaling factors f_{ν} given in the Fig. are only approximately proportional to the ionization energies W_{ν} , and the vertical scaling factors g_{ν} are not well correlated with the number n of electrons. At present it is not known how closely the hydrogenic calculations approximate the correct functions. Because empirical parameters H and V are used in Eq. (5), the degree of approximation cannot be assessed from experimental data for S. More accurate calculations are needed.

Bonderup (1967) derived shell corrections from the stopping power of an electron gas (Lindhard and Winther, 1964) with electron density varying with distance from the nucleus ("local plasma model") and gave functions based on the Lenz-Jensen model. Empirical functions for the shell corrections were given by Andersen and Ziegler (1977) and by Janni (1982). Shell corrections for Au from these sources are shown in Fig. 2.

2. Present approximation.

(a). Inner shells (K, L, M)

The functions given by Walske (1952), Khandelwal (1968), and Bichsel (1983, 1987) were used. The effective charge, Z_ν in Eq. (4a), was assumed to be $n\zeta$, where n is the principal quantum number and ζ the orbital exponent given by Clementi et al. (1967). For the K-shell, $Z_K = Z - 0.3$ was used. The quantities ϵ_ν and W_ν for some elements are given in Table II. From the variations in W_ν for the subshells and from the differences in shape seen in Fig. 1 it is evidently advisable to calculate C_ν for each inner subshell separately.

(b). Outer shells.

From the values of the scaling factors g_ν and f_ν in Fig. 1 we must conclude that for the outer shells there are no compelling choices for the scaling factors H_ν and V_ν in Eq. (5). They must be chosen such as to give good agreement with experimental data.

The ionization energies for the outer shells of some of the heavy elements are given in Table III. In order to reduce the number of free parameters, and in view of the uncertainty of the choice of H_ν , it is reasonable to consider shell correction functions for groups of subshells for which the ionization energies are similar: N_I to N_{III} , N_{IV} and N_V , and all the other shells. I have used this approach and have named the functions C_{N1} , C_{N2} and C_{N3} , using six parameters H_1 , V_1 , H_2 , V_2 and H_3 , V_3 . For the first and second group, the number of electrons in the shells N_I to N_V is constant (18), and we would assume that the factors V_1 and V_2 should change

slowly with Z , at most. It appears plausible to use initial values of H_ν given by

$$H_\nu = J_{M_\mu} \sum \frac{n_\nu}{J_{N_\nu}} / \sum n_\nu \quad [5a]$$

where n_ν is the number of electrons in subshell ν (Table III). I found that values H_1 and H_2 calculated with this Eq. gave better agreement with experimental data for Au than values different by $\pm 20\%$, and no further searches were made with different H_1 and H_2 . Thus there were now only the parameters V_1 and V_2 for which values were undetermined. It was expected though that V_1 and V_2 should be near 1. A further option was the choice of the inner shell μ from which the outer shell functions are scaled. I have found the best agreement with experiments by using the functions C_{MIII} for C_{N2} , C_{MV} for C_{N1} and C_{N3} .

For all electrons outside of N_V (in gold a total of 33 electrons, with ionization energies between 0 and 108 eV) a single function $C_{N3}(v, Z)$ was obtained by scaling C_{MV} with H_3 and V_3 as free parameters (H_3 might be $2H_2$ or greater, and V_3 might be expected to depend on Z).

The method of determining the parameters V_1 , V_2 , V_3 and H_3 is described in section IIH. It will be seen that these four parameters are ample to provide calculated values of the stopping power agreeing well with experimental data.

By choosing the shell corrections to fit experimental data, they will also compensate for errors in L_1 , L_2 and z^* .

D. Barkas and Bloch corrections, L_1 and L_2 .

The need for z^3 and z^4 corrections in the theory was established experimentally by Andersen et al (1977). Basbas (1984) discussed the problem in a general context. Bichsel (1990) analysed experimental data and found that for Au only an empirical function for L_1 approximated experimental data (extending from 1 to 4 MeV) well:

$$L_1(\beta) = 0.002833 \cdot \beta^{-1.2}. \quad [6]$$

Here, this expression has been used for all proton energies, and for all $Z \geq 57$. These extrapolations are dubious.

The term L_2 is written in the form derived by Bloch (1933):

$$L_2 = \psi(1) - \text{Re}[\psi(1+iy)] = -y^2 \sum_{j=1}^{\infty} \frac{1}{j(j^2 + y^2)} \quad [7]$$

where ψ is the logarithmic derivative of the Γ function, and $y = zv_0/v = z\alpha/\beta$ ($\alpha = 1/137.036$ is the fine structure constant). For $y^2 \ll 1$, the sum is equal to 1.202... L_2 does not depend on Z , but does include terms of all even powers of z . Possible errors in L_1 and L_2 will be compensated by the choice of the shell correction parameters.

E. Charge state corrections and nuclear collisions.

Bichsel (1990) found that it was not necessary to use any charge state corrections for protons and α with $T/M \geq 0.5$ MeV (M is the number of nucleons in the ion). For Li-ions, a reduced charge $z^* \leq 3$ appears to be needed for $T/M < 2$ MeV, but no definite form of z^* could be derived from the experiments. For lower energies and heavier ions, the need for charge state corrections will be seen in the Figs. and in Table VIII.

Nuclear collisions contribute less than 0.1% to the stopping power at the energies considered here, and thus are neglected.

F. Mott correction G and density effect, δ .

Ahlen (1978, 1980) gave a close-collision correction $G(z, \beta)$ due to the Mott cross section. For p and α , a rough approximation is $G \approx a_1 z\beta/137$, where $-10 < a_1 < 2$ for $0.3 < T/M < 30$ MeV. Thus this term is less than 0.1% for p and α , but will be more important for heavy ions (e.g. about 2% for 3000 MeV Ca ions).

The algorithm used here for the density effect has been given by Sternheimer et al. (1984). It must be noted that approximations were made which may introduce errors of the order of 0.3% into S_t at $T > 100$ MeV (see Figs. 6.2 to 6.4 in ICRU-37, 1984). The effect amounts to less than 0.04% for 20 MeV protons in gold, and thus is only important for some of the measurements at high energies and for the heavy ions.

G. Ranges and multiple scattering.

Ranges were calculated from stopping power S with the csda (continuous-slowing-down) approximation:

$$R(T) = R(T_1) + \int_{T_1}^T dT' / S(T') \quad [8]$$

For present purposes, for protons, $T_1 = 0.4$ MeV, and $R(T_1)$ was taken as the total pathlength given by Janni (1982). For 10 MeV protons in Au, this contribution amounts to less than 1% of the total range. Due to multiple scattering, experimental projected ranges are shorter than $R(T)$. Corrections for this effect were given by Bichsel and Uehling (1960), Bichsel (1960), Berger and Seltzer (1964), Bichsel (1972), Janni (1982), and by Bichsel and Hiraoka (1989).

H. Method for parameter determination.

The parameters to be determined are the I-value and the scaling factors H_3 and V_ν of Eq. (5) for the outer shell corrections. They were found from experimental data with a least-squares-deviation procedure.

In earlier studies (e.g. Porter and Bryan, 1984), the I-value was introduced explicitly as a free parameter in the data analysis. This can be avoided with the following approach. Customarily, the deviation $\delta(\beta) = L_t(\beta) - L_x(\beta)$ is calculated, and the sum $\sum \delta^2$ is considered as a function of the five parameters. A best fit is obtained if the sum is a minimum. A variation of the parameter I can be avoided if the equation for $\delta(\beta)$ is rearranged as follows:

$$\delta(\beta) + \ln I \equiv Y(\beta) \equiv f_1(\beta) - c_1(\beta) - c_0(\beta) + z L_1(\beta) + L_2(\beta) - L_x(\beta) \quad [9]$$

where $f_1(\beta) = f(\beta) + (G(z, \beta) - \delta(\beta)) / 2$

$$c_1(\beta) = \frac{C_K(\beta) + C_L(\beta) + C_M(\beta)}{Z}$$

$$c_0(\beta) = \frac{C_{N1}(\beta) + C_{N2}(\beta) + C_{N3}(\beta)}{Z} \quad \text{and}$$

the dependence on Z is not indicated. This expression implicitly contains, in $c_0(\beta)$, the four free parameters H_3, V_ν of Eq. (5). If there are no systematic errors in the theory, we expect that $Y(\beta)$ will be a constant (but subject to stochastic errors of the data), and $\exp(Y(\beta)) = I_x(\beta)$ is an experimental I -value for each data point. We define Y_a as the average of p experimental values of $Y(\beta)$:

$$Y_a = \sum_p Y(\beta) / p \quad [10]$$

and by assuming $Y_a = \ln I$, the average deviation σ defined by

$$\sigma^2 = \sum (Y_a - Y(\beta))^2 / (p-1) \quad [10a]$$

is the same as $\sum \delta^2 / (p-1)$. With this approach, the parameter search is performed for a space reduced by one dimension (i.e. a five parameter search is reduced to a four parameter search). σ^2 depends on the parameters H_3, V_ν and can be considered as a function of the four-dimensional space with coordinates H_3, V_ν . The smallest σ^2 define sets of parameters giving best fits to experimental data.

It was found that there were many local minima of σ^2 , and therefore the method of steepest descent was not suitable for the parameter determination; a grid search was used instead. The parameters for small σ^2 were recorded, and the associated functions $Y(\beta)$ were plotted versus particle speed β and examined for systematic deviations. If the deviations ($Y_a - Y(\beta)$) were randomly distributed, or if they deviated systematically by much less than the experimental error, satisfactory values of the four parameters and the corresponding I -value

$$I_a = \exp(Y_a) \quad [10b]$$

had been found. I_a is subject to systematic errors of S_x .

III. EXPERIMENTAL DATA.

For most elements, only the experimental data for protons were used for the parameter determination. The data for α -particles in Au were used implicitly by the determination of the function L_1 for the Barkas effect (Bichsel, 1990). For measurements below 30 MeV, relative to Al or Cu (e.g. Burkig and MacKenzie, 1957), theoretical values from Bichsel (1972) were used to calculate S_x .

I have found that systematic differences occur between experimental data from different sources (see the Figs.) and that the uncertainties σ_e assigned by the authors to their experimental data represent only a qualitative measure of σ_e . This means that a simultaneous χ^2 analysis of several data sets is not practical. Therefore, best fit parameters were determined for each data set, and average values of the parameters were then used. For some data sets where stochastic errors were less than 1% (e.g. Semrad, 1990; Oberlin et al., 1980, 1982; Matteson et al., 1978), a smooth function obtained from a three parameter fit (H_3 , V_3 and I) has been used to represent the data in the Figs.

For gold, I designed an average experimental data set for proton energies above 0.3 MeV. Between 0.3 and 1.5 MeV, data by Luomajärvi (1979), Semrad (1990), Andersen and Nielsen (1981) and Santry and Werner (1981) were used and given about equal weight. Between 1.5 and 3 MeV, the data by Andersen and Nielsen (1981) were reduced by 0.8%. Above 3 MeV, the data by the Nara group (Ishiwari et al., 1984; Shiomi et al., 1986) and those by Sørensen and Andersen (1973) were weighted inversely with their quoted errors. Other data were not used.

For each experimental, $S_x(T)$, and theoretical, $S_t(T)$, value, the relative difference $r(T)$ was determined:

$$r(T) = (S_t(T) - S_x(T)) / S_x(T) \quad [11]$$

Values of $r(T)$, in percent, are plotted in the Figs. The average standard deviation σ_x for an experimental data set with p values was defined by

$$\sigma_x^2 = \sum r(T)^2 / (p-1). \quad [12]$$

$r(T)$ and σ_x should be compared with the errors σ_e of S_x given by the authors, shown in Tables VI, VIII, and in the Figures. If, in general, $|r(T)|$ is less than $|\sigma_e|$, I consider the theory to be adequate. If $|r(T)|$ exceeds $|\sigma_e|$, there may be systematic errors of the theory or the experiments, and the reader is invited to choose which to believe. Symbols used in plotting the data are given in Table V.

IV. RESULTS OF PARAMETER SEARCHES.

A. Shell correction parameters and I-values.

In principle, the parameters could be different for each element. After a preliminary four parameter search for several elements, I found that V_1 and V_2 could be assumed to be constant for all Z . This assumption may have to be changed as more accurate data become available. From an examination of the experimental data I concluded that only for gold there were enough data to permit a meaningful four parameter search. For other elements, a two parameter search for H_3 and V_3 was made, and it was possible to find fixed values of H_3 which were valid for groups of elements. Only for V_3 was it necessary to assume a dependence on Z . Eventually, the I-value resulting from Eq. (10b) was the only truly free parameter.

With the search program based on the use of Eq. (9), uncertainties cannot readily be stated for the parameters (or the stopping power function S_t). It will be seen from Figs. 6-13 that this is not a major problem.

The four parameters V_1 , V_2 , H_3 and V_3 for the outer shell corrections, Eq. (5), were determined for the average data set for gold with the search procedure outlined in section II H. The grid search for local minima of σ^2 , Eq. (10a), was performed with 20 to 30 values of each of the four parameters, with the initial value of H_3 about $1.5 \cdot H_2$, the final value

about $3 \cdot H_2$; the initial V_ν equal to 0.5 and the final values up to 3. In each search, up to 500,000 $\cdot p$ values of S_t were calculated. Results of the search with H_1 and H_2 from Table III are given in Table IV. The 4 parameters V_1 , V_2 , V_3 and H_3 giving a local minimum of σ^2 are listed, together with σ^2 , the I-value and σ_x (Eq. (12)). Since for all these parameter sets the average standard deviation σ_x between experimental and calculated values is less than even the smallest quoted experimental error σ_e ($\pm 0.3\%$), they all could be used to approximate the average data set well. Evidently, this data set is insufficient to determine the parameters uniquely (this of course is also true for the individual sets). Because the number of electrons associated with V_2 is larger than that for V_1 , a value V_2 larger than V_1 is desirable. Thus, the parameters $V_1=1.25$, $V_2=1.4$ are henceforth used for all elements, and the value $H_3=13$ should be valid for elements neighbouring gold in the periodic table.

It is expected that the parameters H_3 and V_3 associated with electrons in the outermost shells (N_{VI} to Q) will depend on the atomic number Z. Therefore I made a two parameter search for H_3 and V_3 for best fits for all elements. I found that for $Z \geq 73$ a value $H_3=13$ gave satisfactory fits; of course, the values V_3 and I varied for each experimental data set. Values of V_3 are plotted in Fig. 3: a tendency toward an increase of V_3 with Z can be discerned, especially for the data from Denmark and Nara. Since V_3 should be related to the number of outermost electrons, $n_o=Z-46$, the function

$$V_3 = (Z-46)/25 \quad [13]$$

was chosen to represent this parameter. The value of V_3 is quite sensitive to experimental uncertainties because C_{N_3} at 1 MeV contributes only about 10% to the stopping number L, Eq. (2), and only 1% at 6 MeV.

For the elements with $57 \leq Z \leq 73$, the results of a two parameter search for H_3 and V_3 are shown in Table VI. Note that σ_x for some data exceeds σ_e slightly. This may mean that the authors underestimate σ_e (see the Figs.). No definite trend of H_3 with Z can be seen, but it appears that a larger value H_3 is appropriate for $Z < 60$ than for $Z > 60$, thus $H_3=50$ and

$H_3=25$ were chosen respectively. For $Z=73$, a smaller value is indicated, and the value for Au ($H_3=13$) was used. Then, a one parameter search was made for V_3 . Values giving best fits are shown in Fig. 4 and in Table VIa, together with I_a and σ_x . Note that σ_x may change little while I_a may change much. This means that the change in H_3 and V_3 is compensated partly by the change in I_a . In Fig. 4, no systematic trend of V_3 with Z can be seen below or above $Z=60$, therefore I chose constant values, approximately equal to the average for all data, viz. $V_3=3.85$ for $Z<60$, $V_3=2.3$ for $Z>60$.

Finally, the average value I_a for each data set was determined with the parameters defined above and the values $b_a=I_a/Z$ are shown in Fig. 5. Again the σ_x are less than σ_e with these I_a for most data sets (Table VIa), and in general they are only slightly larger than σ_x for the one and two parameter fits. The fluctuations in I_a for each Z evidently are in part an expression of the systematic differences between experimental data, but because the values were obtained from data at different energy ranges, they may also indicate possible problems in the assumptions about the theory.

B. Average I-values for the elements.

For the elements with a single data set (Sm, U), the analysis is finished: the experimental value of I for the element is $I_e=I_a$. For elements with several sets of experimental data, we must select a value I_e , a weighted average of I_a (I by the definition of Eq. (2a) is a property of the material). Greater weight was assigned to values from higher energies. The values selected are shown in Table I. They are only valid in the context of the other parameters selected here, and of the experimental data used in the analysis. An uncertainty of I_e of $\pm 1.5\%$ to $\pm 5\%$ should be assumed. A comparison with other experimental values of I is only meaningful to show trends with Z .

It is notable that (except for W, Bi and Th) b_e and the value b_L calculated with the local density model differ by less than $\pm 5\%$ (the average deviation is $(0.6\pm 3.3)\%$), even though b_L was calculated for single atoms, while b_e was

measured for the metal. Some of the variation in b_e must be related to the variation in hf and in the plasmon energy hf_v of the valence electrons. In particular, this may explain the difference in b_e between Au, Pb and Bi. It appears advisable to be suspicious of the values of b_e for W, Bi and Th. Fluctuations in b_e for neighbouring Z may be indicative of systematic errors in the measurements.

The differences between b_e and b_J and b_A are explained in part by the fact that a larger set of data was used here. It must be understood clearly that values b_e will change as further experimental data become available.

The I-values for Pb and U for the proton energies below 30 MeV are less than those indicated from the higher energies. Further studies appear to be needed.

A determination of I-values with an uncertainty of less than 2% from other methods (e.g. Shiles et al., 1980) is highly desirable.

V. Comparison of theory and experiment.

A. Protons.

The comparison between experimental data S_x and theoretical functions S_t for $T \leq 30$ MeV is made in Figs. 6-13. The relative difference $r(T)$, Eq. (11), is shown as a function of kinetic energy T/M of the protons. The authors' experimental uncertainties are shown at only a few energies. There is no evidence to invalidate the theory. It is somewhat surprising that the theory agrees with experiments at energies T well below 1 MeV. There are no general trends for $r(T)$ to be definitely larger than 0, thus no need for a reduced effective charge z^* is evident. For Ta, Fig. 7, the agreement between theory and experiments as well as between different experiments is poor. While the data by Luomajärvi (1979) for p in Ta differ considerably from theory, they agree quite well for W and Au.

Some experimental data not included in the Figs. are considered next. For Th, data by Teasdale (1949), Sonett and MacKenzie (1955) and Burkig and MacKenzie (1957), with $H_3=13$,

$V_3=1.76$ result in $I_a=766$ eV, $\sigma_x=\pm 0.7\%$. Energy loss measurements for protons with initial energies T_i between 14 and 25 MeV in thick absorbers were made by Bichsel and Tschalär in 1966 with the method described by Tschalär (1967) and Tschalär and Bichsel (1968). The residual energies T_f were measured with silicon detectors and corrected for multiple scattering. A theoretical thickness $t_t=R(T_i)-R(T_f)$ was obtained from range energy tables calculated with Eq. (8). The uncertainty of the energy-measurements (less than $\pm 0.1\%$ for T_i , about ± 24 keV for T_f) corresponds to an uncertainty of no more than 0.5% in calculated thicknesses t_t . The results have not been published so far because the theory used in 1967 was inadequate. Experiment and present theory are compared in Table VII. For both metals, a systematic trend with energy is seen. Larger I -values would provide somewhat better agreement.

Sakamoto et al. (1989) measured the stopping power for 73 MeV protons in ten elements with an uncertainty of $\pm 0.7\%$. Data are shown in Table VIII. Only the value for Pb exceeds σ_e significantly. A value $I=855$ eV would be needed to achieve $r=0$ for Pb. For Al, $r=0.3\%$ and for Cu, $r=0.8\%$ from the tables described below.

Several measurements with high energy protons have been reported. They are listed in Table IX. Usually the range of particles with a fixed energy was measured in Al or Cu. Then a given layer in the principal absorber was replaced by another material, and the range measurement was repeated. The ratio of thicknesses of materials causing the same energy loss was thus determined. In order to obtain the stopping power for the second absorber, that of the first absorber must be known. Therefore, stopping power tables for Al and Cu were calculated with the shell corrections given in ICRU-37 (1984), with $I(\text{Al})=166$ eV, $I(\text{Cu})=322$ eV and the density effect of Section II F. No corrections for straggling, multiple and nuclear scattering and nuclear reactions were made beyond those made by the authors. It must be noted that the change in the multiple scattering and the straggling in the second absorber will lead to changes in the total range (of the order of 0.5%) which have not been considered so far (Bichsel and Hiraoka, 1989).

It was found that the ratio of absorber thicknesses even for fairly large energy losses (e.g. $T_i=340$ to $T_f=270$ MeV) differs by no more than 0.1% from the ratio of stopping powers at the mean energy (i.e. 300 MeV). This can readily be confirmed from existing range tables (Bichsel, 1972). Therefore, S_x was calculated from the ratio of thicknesses ("mass stopping power") given by the authors and the theoretical stopping power of the reference material (Al or Cu) at the mean energy T given by the authors.

For Bakker and Segre (1951), $T_i=340$ MeV, $T_f \approx 270$ MeV, $\sigma_e = \pm 1\%$, S_x was calculated with S_t of both Al and Cu, and the average is given in the table. For U, σ_x exceeds σ_e slightly. For the ratio $S_x(\text{Al})/S_x(\text{Cu})$, the difference of 1% may be indicative of systematic errors in theory or measurement.

Barkas and von Friesen (1961) with 750 MeV protons measured thicknesses of several materials relative to the equivalent thicknesses of Cu at several depths in a copper absorber. Theoretical values of the stopping power of Cu were used to obtain S_x for Pb, U and Al. Since the estimated experimental error is considerably less than 1%, the relative differences r between theory and experiment are disturbingly large. Larger I -values would be needed to get $r=0$. If the measurements had been made relative to Al, the average r for Pb would be 0.5%, for U, 0.3%.

Vasilevskii and Prokoshkin (1967) measured stopping power of Pb relative to Cu for p , d and α . The data are listed in Table IX at the equivalent proton energy. The absolute values of S_x given for Cu by these authors (shown in Table IX) were used to calculate S_x for Pb. For Pb, the agreement between theory and experiment is good, but the experimental values for Cu exceed the theoretical values by 0.8% on the average.

Vasilevskii et al. (1969) measured the stopping power of Pb relative to that of Al with the method used by Barkas and von Friesen (1961) with an initial beam energy of 660 MeV. The theoretical stopping power function for Al was used to calculate S_x for Pb. Here, on the average, S_t for Pb exceeds S_x by 1.3%. It is interesting to include the experimental

data for Cu: in contrast to the data by Barkas and von Friesen, there is essentially no difference between theory and experiment.

From the data at energies above 20 MeV, a higher I-value (which would reduce S_t) is indicated for Pb and U. The need for further correction terms in the theory must also be considered.

B. Helium and heavier ions.

Selected data for α are shown in the Figs. and in Table VIII. The values of r generally increase with decreasing $T/M < 0.5$ MeV, indicating the need for a charge state correction.

Since the Barkas correction L_1 was determined from the data for Au by Andersen et al. (1977), we can expect the agreement between S_x and S_t for α to be good. This is indeed the case. Agreement within experimental errors was also found for Li-ions (Bichsel, 1990).

For Au, only the data by Fontell and Luomajärvi (1979) (dashed-dotted line) and by Matteson et al. (1978) (solid line near $T/M=0.5$ MeV) are shown in Fig. 6a. Other data are shown in Table VIII.

For the experimental values by Anthony and Lanford (1982) for C-ions in gold, a charge state correction is needed if it is assumed that L_1 is correct for $z > 3$.

The experimental data by Datz et al. (1977) appear to have large systematic errors. The need for a charge state correction or for changes in L_1, L_2 etc. appears for $z > 4$.

Experimental data by Ishiwari et al. (1971, 1977, 1978) and data by Takahashi et al. (1983) generally agree with theory. For the C-ions, L_1 and L_2 amount to 8% and 5% of L , respectively. The expression given by Eq. (6) seems to be valid for $z=6$ at this energy. The Mott term amounts to less than 0.2%. For Pb, an I-value of 747 eV would give better agreement with experiments.

The data for ^{16}O , ^{36}Ar , ^{40}Ar and ^{40}Ca ions traversing Ta and Au agree well with calculated values, except for O-ions with $T < 100$ MeV in Au, where a charge state correction appears to be necessary. The data at 75 MeV seem to be wrong.

A function correcting for charge state z^* is needed for $T/M < (z-1.5)$ MeV. The data presented here are not sufficient to arrive at a quantitative description of $z^*(\beta)$.

C. Range measurements.

Range data were not suitable for the determination of the shell correction parameters. In principle, I-values could be obtained from them. In Table X, experimental ranges, R_x , are compared with calculated ranges R_t , Eq. (8).

The ranges of protons in Au measured by Bichsel et al. (1957), were corrected by the multiple scattering corrections given by Bichsel and Uehling (1960). They are in good agreement with the theory. Asymmetries in the range-straggling function (Lewis, 1952; Tschalär, 1968; Bichsel and Hiraoka, 1989) have not been taken into account yet.

The ranges for protons in lead measured by Bloembergen and van Heerden (1951) ($\sigma_e \approx \pm 0.5\%$ to $\pm 1\%$) are given uncorrected for multiple scattering. They exceed the calculated values on the average by $(0.2 \pm 0.3)\%$. Since the multiple scattering correction amounts to $\approx 1.7\%$ (Bichsel, 1972), the calculated values are too small by this amount. An I-value of 860 eV would be needed to give calculated ranges agreeing with measured values, corrected for multiple scattering. It must be noted that the multiple scattering corrections given by Janni (1982) are about 50% larger.

The ranges of protons in lead, measured by Mather and Segrè (1951), corrected for multiple scattering (Bichsel, 1960; Berger and Seltzer, 1964) agree well with calculated values. The ranges measured in Al and Cu, though, are 1% and 1.5% less than the theoretical ones.

A range measurement by Vasilevskii and Prokoshkin (1967) for 620 MeV protons in Pb relative to the range in Al exceeds

the calculated range by 1.5%.

The corrected ranges R_x for 750 MeV protons in Pb and U measured relative to the range in Cu by Barkas and von Friesen (1961) exceed the calculated ranges R_t by 1.2%. The range for Al is also given. It agrees well with R_t , in contrast to the data for the stopping powers in Table IX.

We see that for three out of four sets of range measurements for Pb a larger I-value is indicated than from the stopping power data.

VI. USE OF THE THEORY FOR LOW ENERGIES.

The expression for the stopping number L of Eq. (2) contains several terms which change quite rapidly with particle energy at small speeds. This can be seen in Table XI, where the terms of Eqs. (2) and (2a) are shown for protons in gold. The shell corrections are combined into "inner shells", c_i and "outer shells" c_o (Eq. (9)). The high speed approximation is defined by $L_B = f(\beta) - \ln I$, usually called the "Bethe approximation". For $E > 1$ MeV, L_B differs by no more than 10% from L , but the sum of the corrections still amounts to 1.5% at 100 MeV (the Mott term G and the density correction δ amount to less than 0.1% and are included in $f(\beta)$).

With decreasing energy, the various correction terms begin to contribute increasing amounts to L . Around 1 MeV, the net contribution from the shell corrections, $c_i + c_o$, is almost zero. Below about 0.5 MeV, the major contribution to L is from c_i ! Clearly, the values for L below about 3 MeV depend strongly on the values of the parameters used, and it is quite remarkable that most experimental data agree well with theoretical values at small energies for protons as well as for α .

All the terms in Eqs. (2) and (2a) have a well defined physical meaning even at the smallest energies listed here, and therefore, no definite energy can be given at which the theory is invalid. On the other hand, the magnitude of each of the terms is not well determined theoretically. If for

example different functions were used for L_1 and L_2 , changes in H_ν and V_ν could compensate for most changes. For heavier ions, deviations between theory and experiment would be accommodated by a charge state correction which would require further free parameters.

VII. TABLES OF STOPPING POWER.

Values of stopping power for p and α calculated with the present theory are given in Tables XII and XIII. They are compared with other tabulations in Fig. 14. Andersen and Ziegler (1977) published an evaluation of experimental stopping power data for protons. For energies greater than 1 MeV, they used six free parameters to calculate the stopping power (see their Table 1, p.16: the parameter $A_6 = 5.099 \cdot 10^{-4} Z$ is not a free parameter; $A_7 = 2mc^2 / I$ is a free parameter and corresponds to I_e in the present paper; the other five parameters, A_8 to A_{12} , show a systematic dependence on Z , but are not related to the parameters H_ν and V_ν used here). For $E < 1$ MeV, four parameters were used.

Janni (1982) gave stopping powers for protons. He used the scaling procedure of Eq. (5) to obtain shell corrections for each subshell from Walske's (1956) L-shell corrections. Data from the tables by Williamson et al. (1966) are also shown in Fig. 14. Data for p in Pb above 1 MeV in Bichsel (1972) differ by less than 1% from present values. A major reason for the relatively large differences below 2 MeV is the inclusion in the present study of the data by Knudsen et al. (1980), Sirotinin et al. (1984) and Luomajärvi (1979) (see Table VI) which were not available for the earlier evaluations.

For all the tables, the differences seen in Fig. 14 are in part due to differences in the choice of the I -values (see Tables I and X), but there are also considerable differences in the shell corrections (see Fig. 2).

A comparison of the proton stopping power tables of Andersen and Ziegler (1977) and the tables for α particles by Ziegler (1977) was made by Bichsel (1990).

VIII. CONCLUSIONS.

Initially, the theory presented here contained seven free parameters: H_ν and V_ν , $\nu=1,2,3$ and I_a , in addition to the choice of Z_ν for the L- and M-shells (see Table II). After preliminary searches, H_1 and H_2 were chosen according to Table III, while V_1 and V_2 were determined in parameter searches from the averaged data for protons traversing gold, and were assumed to be constant for the other elements. Finally it was found that constant values of H_3 , for groups of elements, with V_3 given as a function of Z , and I_a as the only free parameter gave good agreement with experiments for protons, α -particles (Figs. 9-13) and some heavier ions (Table VIII) for all elements with $Z \geq 57$. For gold, I estimate the uncertainty of the theory to be $\pm 1\%$ below 3 MeV, $\pm 0.5\%$ between 3 and 20 MeV, 1% above 20 MeV. For other elements, it may be ± 2 to 3% below 3 MeV, $\pm 1\%$ above. The influence of the uncertainty of the I -value must be added. For $T > 30$ MeV, further correction terms may be needed.

The present approach is plausible insofar as it includes all of the elements of current thoughts about Bethe-Bloch theory. It relies heavily on the experimental data for the determination of the parameters though. In examining the data for individual experiments for various Z in Tables VI and VIA it is seen that a single experimental data set cannot be expected to provide the parameters H_3 , V_3 and I_a suitable for other data. Thus it appears inadvisable to determine parameters on the basis of data for a single data set, especially if they extend over a restricted energy range; and earlier studies (e.g. Bichsel, 1967; Porter and Bryan, 1980) are only applicable for the particular sets of experimental data used in their analysis.

If the theory is to be used for elements not listed in Table I, an I -value must be chosen. This could be done, e.g., by using b_e from a neighbouring element or a calculated value of b_L .

Many systematic errors of unknown magnitude are associated with the theoretical functions used here. Examples are:

1. use of nonrelativistic hydrogenic wave-functions (Appendix),
2. use of scaling procedure for the calculation of the shell corrections,
3. extrapolation of empirical L_1 to lower energies and different Z,
4. influence of the approximations used by Bloch in his derivation of L_2 ,
5. neglect of higher terms in the Born approximation,
6. approximations used for the Mott term and the density effect,
7. neglect of charge exchange effects (e.g. Arnau et al., 1990).

In addition, systematic errors of the experimental data cannot necessarily be discerned. An example is the modification of the Andersen et al. (1977) data for Au by Andersen and Nielsen (1981). Therefore the results for I_e based on a single set of data (i.e. Ce, Pr, Sm, Ho, Th, U) must be considered to be tentative. Furthermore, the results for Ta (Fig. 7) do not inspire much trust in the experiments or the theory. Only the results for Au and maybe Pb can be considered more than tentative. I would be surprised though if new measurements would show the need for changes in the basic parameters of Tables II and III, and in V_1 and V_2 . Measurements for proton energies between 0.5 and 6 MeV for several elements with an uncertainty of no more than 0.3% would demonstrate the Z-dependence of H_3 and V_3 more clearly. Similar measurements would be required to establish values of H_3 , V_3 and I for compounds.

Further developments of the theory appear to be tedious and may not be worthwhile unless further measurements show a need for them. A better approximation for L_1 could be determined by measurements at $0.5 \leq T/M \leq 2$ MeV at least for protons and α -particles with an error of less than 0.3%.

The independent determination of I-values from Eq. (3) with an uncertainty of less than $\pm 2\%$ is desirable (it would help e.g. with the problems with the data for Ta). Accurate X-ray absorption measurements and electron energy-loss data similar to those by Ahn et al. (1983) would be needed for

this purpose. Such I-values would also help in establishing the errors of the scaling factors H_ν and V_ν - or they might demolish the present approach.

While approximations better than the nonrelativistic hydrogenic calculations for K- and L-shell excitations have been made for collision cross sections (reviewed e.g. by Cohen and Harrigan, 1985), these calculations still differ by large amounts from experimental data at low particle speeds. It is thus an open question whether corresponding calculations for the shell corrections would be helpful.

It should be explored whether the differences between theory and experiments for stopping powers and ranges at energies above 30 MeV indicate the need for further correction terms in the theory.

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APPENDIX: RELATIVISTIC EFFECTS IN ABSORBER ATOM.

Leung (1989) described a correction to the Bethe theory which he obtained from considering relativistic effects for the atomic electrons. For Au, he estimated an increase of S of about 2% due to this effect. The change was related to relativistic corrections to the Bethe sum rule described by Rustgi et al. (1988). The introduction of this correction term into the present analysis [with the expression given in Leung's Eqs. (13) and (14)] changes the coefficients H and V for outer shell electrons, and decreases the I -values. For an average data set for Pb, consisting of the data by Ishiwari et al. (1984) and Sørensen and Andersen (1973), the following three parameter best fit was obtained: $H_3=12$, $V_3=2$ and $I=720$ eV, with $\sigma_x=\pm 0.08\%$. The fit is as good as that shown in Fig. 7. If these parameter values are used for all the high energy data for Pb, the average value of r is $(0.2\pm 0.9)\%$, compared to $(1.4\pm 0.9)\%$ for the standard parameters. Thus the Leung correction to the stopping power function brings the theory into closer agreement with experiment at the higher energies, and it appears desirable to explore this effect in more accurate studies. Also, more accurate measurements at both low and high energies would be useful to assess the accuracy of this correction.

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Ziegler, J. F., 1977, "Helium stopping powers and ranges for all elemental matter", Pergamon Press, New York. In Table 1 (p.55) of this ref., the values of S_e for $Z > 72$ and for $10 < E/\text{MeV} \leq 30$ seem to be too small by up to 15%.

TABLE I. Values of Bloch parameters $b=I/Z$ from various sources, and related quantities (section IIB): average experimental plasmon energies, hf_v and plasma energies hf , all in eV. b_L was calculated for atoms with a local density model, b_e is the experimental value from Table V and Fig. 5; and b_S was calculated from ionization energies. Values used in other tabulations are: b_J (Janni, 1982); b_A (Andersen and Ziegler, 1977); b_I (ICRU, 1984). They differ from b_e partly because different shell corrections and different experimental data sets were used, partly because different assumptions about the dependence on Z were used.

Z		hf_v	hf	b_L	b_e	b_S	b_J	b_A	b_I
57	La	-	45.9	8.53	8.32	11.8	9.75	8.42	8.8
58	Ce	-	48.2	8.6	8.76	-	9.75	8.5	8.8
59	Pr	-	48.5	8.67	8.64	11.2	9.76	8.59	9.1
62	Sm	-	50.6	9.04	9.05	10.0	9.78	8.84	9.78
64	Gd	-	51.5	9.08	8.83	9.0	9.27	8.81	9.2
66	Dy	-	53.7	9.4	9.17	9.1	9.8	9.09	9.8
67	Ho	-	54.5	9.36	9.55	-	9.8	9.3	9.8
68	Er	-	55.6	9.6	9.56	8.6	9.11	9.41	9.7
70	Yb	-	48.3	9.65	9.66	7.6	9.82	9.46	9.82
72	Hf	-	66.2	9.76	9.32	-	9.83	9.47	9.83
73	Ta	-	74.6	9.78	10.05	9.2	10.11	9.37	9.8
74	W	25	80.3	9.8	10.53	9.6	10.17	9.36	9.8
77	Ir	-	86.5	9.87	10.23	-	9.93	9.55	9.8
78	Pt	23	84.2	9.96	10.08	9.8	10.58	9.73	10.1
79	Au	24	80.2	10	10	9.9	10.21	9.56	10
82	Pb	15	61.1	9.79	9.5	10.7	9.99	9.26	10
83	Bi	18	56.9	9.71	8.98	-	9.87	9.22	9.9
90	Th	-	61.3	9.06	8.51	-	8.18	9.17	9.4
92	U	-	77.4	9.16	9.09	14	9.56	9.21	9.7

TABLE II. Parameters used for the calculation of shell corrections for the L- and M-shells for some heavy elements. n_{ν} is the number of electrons in each subshell. The total number of electrons included in these shells is 26. In the first line for each element, the value of the atomic unit for each subshell, defined by $\epsilon_{\nu} = Ry \cdot Z_{\nu}^2$, Eq. (4a), is given in keV. In the second line, the ionization energy is given in atomic units, $W_m = J_{\nu} / \epsilon_{\nu}$, where J_{ν} is the measured ionization energy found in Bearden and Burr (1967).

shell	L _I	L _{II}	L _{III}	M _I	M _{II}	M _{III}	M _{IV}	M _V
n_{ν}	2	2	4	2	2	4	4	6
element								
La	23.94	37.91	37.91	19.57	19.78	19.78	25.22	25.22
57	0.262	0.155	0.145	0.07	0.061	0.057	0.034	0.033
Gd	30.32	48.48	48.48	25.98	26.51	26.51	34.38	34.38
64	0.276	0.164	0.149	0.072	0.064	0.058	0.035	0.034
Ta	39.55	63.97	63.97	35.5	36.49	36.49	48.05	48.05
73	0.295	0.174	0.154	0.076	0.068	0.06	0.037	0.036
Au	46.34	75.51	75.51	42.29	43.73	43.73	58.36	58.36
79	0.31	0.182	0.158	0.081	0.072	0.063	0.039	0.038
Pb	49.66	81.63	81.63	45.99	47.58	47.58	63.9	63.9
82	0.319	0.186	0.16	0.084	0.075	0.064	0.04	0.039
U	60.21	99.65	99.65	56	58.49	58.49	80.4	80.4
92	0.361	0.21	0.172	0.096	0.085	0.071	0.045	0.044

TABLE III. Ionization energies J_ν (Bearden and Burr, 1961) and horizontal scaling factors H_1 and H_2 for the calculation, Eq. (5), of the shell corrections C_{N1} (the average value for the 8 electrons in shells N_I to N_{III}) and C_{N2} (for the 10 electrons in shells N_{IV} and N_V). Values of H_1 and H_2 are defined by the average value of the ratios $J_{MV} / J_{N\nu}$, weighted with number n_ν of electrons in each subshell.

shell	M_V	N_I	N_{II}	N_{III}	N_{IV}	N_V	H_1	H_2	
n_ν	6	2	2	4	4	6			
element			J_ν (eV)						
La	832	270	206	191	99	99	3.96	8.4	
Gd	1185	376	289	271	141	141	4	8.4	
Er	1409	449	366	320	177	168	3.94	8.22	
Ta	1735	566	465	404	241	229	3.84	7.43	
Au	2206	759	644	545	352	334	3.6	6.47	
Pb	2484	894	764	644	435	413	3.43	5.89	
U	3552	1441	1273	1045	780	738	3.01	4.71	

TABLE IV. Parameters V_1 , V_2 , H_3 and V_3 for local best fits to the average data set for protons in gold, obtained in a four parameter grid search. $H_1=3.6$ and $H_2=6.47$ are given in Table II. σ^2 is defined in Eq. (10a), σ_x in Eq. (12), and $I_a = \exp(Y_a)$ [Eq. (10)]. A local best fit is defined as a local minimum of σ^2 in the four dimensional space defined by V_1 , V_2 , V_3 and H_3 . Note that the smallest values of σ_x do not necessarily occur at the same grid-point as the smallest values of σ^2 . This is because of the nonlinear relation between $\ln I$ and S .

V_1	V_2	H_3	V_3	σ^2	I_a/eV	σ_x %
1.3	1.1	12.8	1.35	0.01494	792	0.1525
1.3	1.15	13.	1.35	0.01466	791.4	0.1555
1.3	1.2	13.	1.35	0.01511	790.3	0.1602
1.3	1.25	13.2	1.35	0.01631	789.7	0.1686
1.3	1.3	13.4	1.3	0.01645	790.9	0.1678
1.25	1.35	12.8	1.3	0.01498	791.3	0.1633
1.25	1.4	13.	1.3	0.01429	790.7	0.1571
1.25	1.45	13.2	1.3	0.01459	790	0.1613
1.25	1.5	13.4	1.3	0.01579	789.3	0.1737
1.2	1.55	12.8	1.25	0.01674	791.7	0.1684
1.2	1.6	13.	1.25	0.01513	791	0.159
1.2	1.65	13.2	1.25	0.01448	790.3	0.1588
1.2	1.7	13.2	1.25	0.01447	789.3	0.1677
1.2	1.75	13.4	1.25	0.01532	788.6	0.172
1.2	1.8	13.6	1.25	0.01696	787.9	0.1822
1.15	1.85	13.	1.2	0.01541	790.3	0.1745
1.15	1.9	13.2	1.2	0.01443	789.6	0.1676
1.15	1.95	13.4	1.2	0.01433	788.9	0.1678
1.15	2.	13.6	1.2	0.01503	788.2	0.174

Table V. Symbols used for plotting data in Figs. 3-13

Reference	symbol
Oberlin (1980, 1982), Luomajarvi (1979)	×
Bader (1956), Borders (1974)	◇
Langley (1976), Santry (1984)	□
Knudsen (1980), Green (1955), Chumanov (1979)	+
Nara	⋈
UCLA, Lin (1973)	⊕
DK, Fontell (1979)	⊗
Semrad (1990), Chu (1973)	✱
Sirotnin (1984), Kuldeep (1985)	○

Nara: Ishiwari (1984, 1988), Sakamoto (1986), Shiomi (1986)
 UCLA: Teasdale(1949), Sonett(1955), Burkig(1957), Nakano(1963)
 DK: Sørensen (1973), Andersen (1967, 1969, 1981)

TABLE VI. Best fit values of H_3 and V_3 for $57 \leq Z \leq 73$, obtained in a two parameter search for $^3\text{protons}$ with $T > 0.3$ MeV and α with $T > 1.6$ MeV with $V_1 = 1.25$ and $V_2 = 1.4$, and H_1 and H_2 from Table III. σ_x is defined by Eq. (12), I_a by Eq. (10b). If $V_3 = 0$, H_3 is indeterminate. The experimental errors σ_e are those given by the authors (for some, an average value is given). Authors: A: Andersen et al. (1969); B: Bader et al. (1956); Bo: Borders (1974); C: Chu et al. (1973); G: Green et al. (1955); K: Knudsen et al. (1980); L: Luomajärvi (1979); La: Langley and Blewer (1976); N: Ishiwari et al. (1988); O: Oberlin et al. (1980, 1982); P: Lin et al. (1973, 1974); S: Sirotinin et al. (1984); U: Teasdale (1949), Sonett and MacKenzie (1955), Burkig and MacKenzie (1957) and Nakano et al. (1963).

Z	set	σ_e	H_3	V_3	$\sigma_x \%$	I_a / eV
57	La K	2.	78	4.7	2.2	490
	S	3.	46.6	4.47	0.9	462
58	Ce K	4.	75	4.8	3.4	519
59	Pr K	3.	27	3.75	2.4	456
62	Sm S	3.	18	2.2	3.4	548
64	Gd K	2.	48	3.1	1	582
	S	3.	22.5	2.7	3.2	542
	A	0.6	--	0	0.35	587
	α O	3.	79	4.9	0.3	591
66	Dy K	2.	21	3.3	0.7	531
	α P	4.	19	3.6	2.5	548
67	Ho K	2.5	18.9	3.58	2.5	548
68	Er K	3.	230	10	2.8	679
	O	3.	33	1.3	1.0	691
	La	2.	10	2.5	1.3	604
	α O	2.	18	2.1	0.4	627
70	Yb K	2.	48.	2.5	2.	709
	S	3.	18.	2.15	2.2	678
72	Hf S	3.	17	3.5	1.6	600

73	Ta	B	3.	10.	0.6	0.3	795
		L	2.7	16.	1.3	0.6	744
		A	0.6	10.	0.6	0.	712
		S	3.	15.5	2.2	1.4	706
		U	-	-	0.	1.2	741
		N	0.3	14.5	0.7	0.1	737
	α	P	4.	21.5	1.5	0.	758

TABLE VIa. Best fit values of V_3 for some Z obtained in a one parameter search for protons with $T \geq 0.3$ MeV, α with $T \geq 1.6$ MeV with $V_1 = 1.25$ and $V_2 = 1.4$, H_1 and H_2 from Table II and $H_3 = 50$ for $Z < 60$, $H_3 = 25$ for $60 \leq Z \leq 72$, $H_3 = 13$ for $Z \geq 73$. The values of V_3 are shown in Fig. 4. σ_x and I_a are given. In the last two cols., average I-values, \bar{I}_a (Eq. (10b)) are given, for $V_3 = 3.85$ for $Z < 60$, $V_3 = 2.3$ for $60 < Z \leq 72$, $V_3 = (Z-46)/25$ for $Z \geq 73$. σ_x^3 is also shown. The latter I_a are also shown in Fig. 5.

Z	set	V_3	σ_x	I_a /eV	σ_x	I_a /eV	
57	La	K	3.25	2.1	484	3.1	473
	S		4.8	0.9	462	2.	472
	α	P	4	0.	460	0.1	463
	α	K	6.9	0.	433	2.1	487
58	Ce	K	3.05	3.4	519	3.6	507
	α		K				2.4
59	Pr	K	4.4	2.9	491	3.1	502
	α		K	7.6	0	451	2.9
62	Sm	S	2.4	3.6	558	3.6	561
64	Gd	K	2.45	1.6	555	1.8	561
	S		2.85	3.2	543	3.8	560
	A	0	0.35	587	0.8	576	
	α	O	2.25	0.4	560	0.4	558
	α	K	1.8	0.	600	0.5	573
	α	C					548
66	Dy	K	2.75	1.8	567	1.9	588
	α		P	2.2	0.1	609	0.1
	α	K	2.6	0.	605	0.4	622
67	Ho	K	3.1	3.3	597	3.3	632
	α		K	1.3	0.	719	1.1

68 Er	K	2.	4.3	635	4.1	620
	O	1.3	1.4	682	2.1	650
	La	2.2	2.	674	2.1	671
	α K	0	1.5	785	2.7	633
	α O	1.8	0.5	666	0.8	640
	α La	2.8	0	608	0.5	635
70 Yb	K	2.35	0.8	665	0.7	667
	S	2	3.	698	4.1	684
	α K	0.	2.7	860	4.4	691
72 Hf	S	3.25	3.8	630	3.2	671
	α C					683
73 Ta	B	1.1	0.5	751	0.5	752
	L	1.6	0.4	716	0.8	751
	A	0.8	0.05	712	0.2	707
	S	2.3	2.9	697	3.7	760
	U	0	1.2	741	1.3	735
	N	0.5	0.1	738	0.1	733
	α P	0.	0.5	884	0.7	787
82 Pb	B	2.0	1.0	709	1.3	743
	G	2.9	1.7	652	2	753
	A	1.4	0.1	781	0.12	779
	S	1.6	3	782	3.0	794
	U	0	0.8	832	1.2	816
	N	1.5	0.1	776	0.1	776
	α Bo	0.7	0.9	850	1.	792

TABLE VII. Energy loss measurements in thick absorbers with absolute energy measurements: Bichsel and Tschalär (1966). Initial energy T_i and final energy T_f in MeV. The experimental absorber thicknesses are $t_x=0.5385$ g/cm² for Pt, $t_x=0.5034$ g/cm² for Au. The theoretical absorber thicknesses t_t (g/cm²) were obtained from ranges calculated with Eq. (8), and $\Delta=(t_x - t_t) / t_t$. A larger I-value would increase t_t . For a linear regression fit to $\Delta(t_t)$, the statistical fluctuation of Δ is $\pm 0.2\%$.

	T_i	T_f	t_t	$\Delta(\%)$
Pt	14.364	4.104	0.5379	0.11
	14.416	4.223	0.5378	0.13
	14.538	4.477	0.5380	0.1
	14.735	4.909	0.5370	0.28
	14.761	4.964	0.5368	0.31
	15.258	5.952	0.5354	0.58
	15.778	6.881	0.5352	0.62
	16.315	7.785	0.5349	0.68
	16.811	8.585	0.5343	0.78
	17.507	9.651	0.5340	0.84
	18.329	10.866	0.5329	1.06
	19.198	12.068	0.5335	0.95
	20.021	13.192	0.5325	1.12
	20.909	14.361	0.5322	1.19
	21.961	15.703	0.5322	1.18
	23.045	17.052	0.5323	1.17
	24.129	18.371	0.5326	1.11
	25.243	19.726	0.5308	1.45
	25.433	19.919	0.5337	0.9
Au	14.011	4.354	0.5045	-0.22
	14.503	5.339	0.5042	-0.15
	15.004	6.252	0.5041	-0.14
	15.513	7.145	0.5031	0.06
	16.16	8.19	0.5029	0.09
	16.821	9.204	0.5026	0.15
	17.631	10.394	0.5022	0.25
	18.459	11.553	0.5020	0.27
	19.306	12.719	0.5005	0.58
	20.171	13.845	0.5009	0.5
	21.055	14.976	0.5009	0.5
	21.957	16.117	0.4999	0.71
	22.569	16.888	0.4984	1.0

TABLE VIII. Comparison of calculated, S_t , and measured stopping power, S_x (MeV cm² /g). The kinetic energy, T, of the particles is given in MeV, the authors' experimental accuracy is σ_e , and r(%) is the relative difference, Eq.(11).

1 st auth	part	Z	T(MeV)	$S_x \pm \sigma_e$ (%)	S_t	r%
Sakamoto 1989	p	Ta	70	4.579 ± 0.7	4.618	0.9
		Pt	"	4.508 ± 0.7	4.511	0.1
		Au	"	4.491 ± 0.7	4.518	0.6
		Pb	"	4.388 ± 0.7	4.469	1.9
Chu 1973	α	Ta	2	366 ± 3	378	3
		Au	"	358 ± 3	347	-3
		Pb	"	363 ± 3	348	-4
Santry 1981	He ³	Au	1.0	377 ± 5%	408	8
			1.2	363	380	5
			1.4	348	357	2.6
			1.6	332	338	2
			1.8	315	322	2
2.0	301	309	2.6			
Santry 1980	He ⁴	Au	1.0	390 ± 4%	454	16
			1.2	380	424	12
			1.4	368	399	8
			1.6	355	379	7
			1.8	344	362	5
2.0	331	347	5			
Santry 1979	He ⁴	Au	3.08	285 ± 8%	290	0.4
			5.49	228 ± 6%	223	-2.2
Santry 1984	α	Au	3.18	285 ± 4%	286	0.4
			4.78	242	238	-1.7
			5.16	235	230	-2.2
			5.49	228	223	-2.2
			5.8	221	217	-1.8
			6	221	214	-3
7.69	207	189	-9			
Datz	p	Au	2	43.9 ± 0.8%	45.6	3.8
			8	180	185	2.9
			18	405	419.5	3.6
			50	1057	1146	8
			72	1429	1627	14
			98	1896	2257	19
			128	2259	2815	25
	α	Au	3.5	31.6 ± 0.6%	33.9	7.4
			14	130.4	137.2	5.2

	Li		31.5	292	311	6.7
	B		87.5	810	861	6.3
Anthony 1982	C	Au	28.2	1300 ±2%	1509	16
			33.6	1250 ±3%	1383	11
			39.6	1180 ±3%	1270	8
Ishiwari 1971, 1977 1978	α	Ta	8.05	199.7 ±0.3	193.9	-2.9
			28.2	93.46 ±1	93.43	0
			28.27	93.1 ±0.5	93.28	0.2
		Au	28.21	90.13 ±1	90.17	0
			28.28	91.18 ±0.5	90.04	-1.2
Takahashi 1983	α	Au	20.6	110 ±0.7	109.4	-0.5
			27.63	92.8 ±0.75	91.35	-1.6
	C		61.79	961 ±0.7	989	2.9
			82.9	839 ±0.7	828	-1.3
	α	Pb	21.65	106 ±0.9	105.1	-0.8
			28.59	89.5 ±0.9	88.47	-1.1
	C		64.94	982 ±0.7	951	-3.2
			85.78	814 ±0.7	802.6	-1.4
Bimbot 1978	O	Au	70.24	1720 ±3	1901	10
			74.88	1350 ±6	1835	36
			75.52	1350 ±5	1826	35
			92.64	1560 ±4	1625	4
			96.16	1450 ±8	1589	10
			96.96	1480 ±9	1582	7
Gauvin 1987	O	Ta	393	646 ±1.2	649	0.5
			417	620 ±1.7	623	0.5
			431	600 ±1.7	608	1.3
			723	419 ±1.4	419	0
			762	399 ±1.8	404	1.2
			773	400 ±2.5	400	0
			1418	263 ±1.5	260	-1.1
			1453	257 ±2.3	255	-0.8
		Au	396	616 ±1.3	629	2.1
			421	600 ±1.7	602	0.3
			433	590 ±1.7	591	0.2
			713	412 ±1.5	414	0.5
			754	391 ±1.8	398	1.8
			774	390 ±2.5	390	0
			1350	263 ±1.1	263	0
			1429	259 ±1.5	253	-2.3
Bimbot 1986	Ar	Ta	1018	3050 ±1	3170	4
			1063	2920 ±3	3076	5
			1072	3080 ±4	3058	-0.7
			2300	1800 ±1.7	1794	-0.3

			2342	1750 ±2.3	1771	1.2
	Au		935	3110 ±1.3	3268	5
			1027	3050 ±1.6	3067	0.6
			1059	2880 ±3	3004	4
			1073	2800 ±4	2978	6
			1532	2330 ±1	2329	0
			1653	2150 ±1.5	2209	2.7
			1718	2100 ±2.4	2151	2.4
			2157	1810 ±2.8	1834	1.3
			2301	1730 ±2.3	1753	1.3
			2356	1760 ±2.8	1725	-2
			2957	1440 ±1.4	1472	2.2
			3028	1400 ±2.9	1448	3.4
	Ca	Au	2919	1830 ±1.1	1834	0.2
			3010	1750 ±2.3	1796	2.6
Schwab 1989	Ar	Pt	2912	1366 ±0.6	1381	1.1
		Au	2402	1556 ±0.1	1581	1.6
			2650	1451 ±0.3	1477	1.8
			3005	1367 ±0.8	1354	-1

TABLE IX. Measurements of energy loss relative to Al or Cu. The theoretical values of S for Al and Cu are given. The Barkas and von Friesen (1961) data for Al alloy have been converted to pure Al₂. The energy T is the average between T_i and T_f. S in MeV cm²/g, r given by Eq. (11). Theoretical S_t for Al and Cu are given for reference. Barkas data are for pure Al (ICRU 1984).

First author	Z	T/MeV	S _x ±σ _e %	S _t	r %
Bakker	W	300	1.874 ±1	1.858	-0.9
	Pb	"	1.819 ±1	1.827	0.4
	U	"	1.736 ±1	1.758	1.3
	ratio Al/Cu	"	1.143 ±1	1.155	1.1
Barkas	Pb	380	1.606	1.627	1.3
		530	1.391	1.419	2
		680	1.277	1.307	2.3
	U	380	1.548	1.567	1.2
		530	1.353	1.365	0.9
		680	1.24	1.258	1.4
	Al	380	2.415	2.451	1.5
		530	2.089	2.116	1.3
		680	1.913	1.936	1.2
	Cu	380	-	2.126	
		530	-	1.837	
		680	-	1.681	
Vasilevskii 1967	Pb	173.9	2.496 ±0.8	2.496	0
		188.5	2.347 ±0.8	2.376	1.2
		615	1.345 ±0.8	1.348	0.2
		650	1.332 ±1.3	1.325	-0.5
	Cu	173.9	3.332 ±0.5	3.32	-0.3
		188.5	3.142 ±0.5	3.154	0.4
		615	1.765 ±0.6	1.739	-1.5
		650	1.734 ±1.0	1.706	-1.6
Vasilevskii 1969	Pb	110	3.314 ±0.8	3.364	1.5
		300	1.804 ±0.6	1.827	1.3
		420	1.531 ±0.6	1.557	1.7
		600	1.343 ±0.5	1.359	1.2
	Cu	110	4.51 ±0.8	4.53	0.4
		300	2.405 ±0.6	2.399	-0.2
		420	2.029 ±0.6	2.028	0
		600	1.761 ±0.5	1.754	-0.4

TABLE X. Comparison of experimental ranges R_x to theoretical ranges R_t (g/cm_2). The kinetic energy of the incident particles is T^2 (MeV), $\Delta R = R_x - R_t$. Except for the Bloembergen and van Heerden (1951) data, the experimental ranges have been corrected for multiple scattering.

1 st author	Z	T (MeV)	$R_x \pm \sigma_e \%$	R_t	$\Delta R/R \%$
Bichsel 1957	Au	9.698	0.3316	0.3324	-0.25
		17.549	0.8685	0.8667	0.2
Bloembergen 1951	Pb	62.5	7.41	7.375	0.5
		72.1	9.4	9.404	0
		78.9	11.01	10.96	0.4
		82.4	11.82	11.8	0.1
		89.1	13.5	13.48	0.1
		95.3	15.15	15.12	0.2
		104.1	17.58	17.57	0.1
		106.6	18.28	18.29	0
114.1	20.7	20.52	0.9		
Mather 1951	Pb	338.5	123.25	123.88	-0.5
		339.7	124.61	124.58	0
	Cu	339.7	92.69	93.65	-1.0
	Al	339.7	79.42	80.6	-1.5
Vasilevskii 1969	Pb	620	318.2	313.4	1.5
	Al	620	-	206.1	-
Barkas 1961	Pb	750	417.7	413.0	1.1
	U	750	434.7	429.2	1.3
	Al	750	274.7	274.1	0.2
	Cu	750	-	316.5	-

TABLE XI. Contributions to the stopping number, L , Eqs. (2) for protons of energy T (MeV) passing through a gold absorber with $I=790$ eV, $\ln I = 6.672$. $L_B = f(\beta) - \ln I$. The shell corrections, c_1 and c_0 are defined in Eq. (9), L_1 in Eq. (6), and L_2 in Eq. (7). The density effect is included in $f(\beta)$, it amounts to 0.062 at 100 MeV. Note that a fractional change of $Y\%$ in L (or S) causes a change of $(YL)\%$ in the I -value.

T	L	L_B	$f(\beta)$	c_1	c_0	L_1	$-L_2$
0.30	0.5374	-0.1901	6.4819	-0.6270	0.0398	0.2338	0.0935
0.40	0.6374	0.0974	6.7695	-0.5398	0.1252	0.1968	0.0713
0.50	0.7273	0.3204	6.9924	-0.4724	0.1800	0.1721	0.0577
0.60	0.8097	0.5026	7.1746	-0.4175	0.2163	0.1543	0.0484
0.70	0.8862	0.6565	7.3286	-0.3714	0.2408	0.1407	0.0417
0.80	0.9575	0.7899	7.4619	-0.3317	0.2573	0.1299	0.0366
0.90	1.0245	0.9075	7.5796	-0.2969	0.2683	0.1210	0.0326
1.00	1.0876	1.0127	7.6848	-0.2662	0.2755	0.1136	0.0295
1.10	1.1472	1.1079	7.7799	-0.2386	0.2798	0.1073	0.0268
1.20	1.2037	1.1947	7.8667	-0.2138	0.2820	0.1019	0.0246
1.30	1.2574	1.2746	7.9466	-0.1912	0.2828	0.0971	0.0228
1.40	1.3083	1.3485	8.0206	-0.1703	0.2823	0.0929	0.0212
1.50	1.3573	1.4174	8.0894	-0.1515	0.2809	0.0891	0.0198
1.60	1.4041	1.4817	8.1538	-0.1341	0.2790	0.0857	0.0186
1.70	1.4489	1.5422	8.2142	-0.1180	0.2765	0.0827	0.0175
1.80	1.4920	1.5992	8.2712	-0.1031	0.2736	0.0799	0.0165
1.90	1.5334	1.6531	8.3251	-0.0891	0.2705	0.0774	0.0157
2.00	1.5732	1.7042	8.3763	-0.0761	0.2672	0.0750	0.0149
2.50	1.7533	1.9265	8.5986	-0.0221	0.2491	0.0657	0.0120
3.00	1.9080	2.1080	8.7801	0.0181	0.2309	0.0589	0.0100
3.50	2.0437	2.2614	8.9334	0.0490	0.2137	0.0537	0.0086
4.00	2.1648	2.3941	9.0661	0.0733	0.1981	0.0496	0.0075
5.00	2.3737	2.6156	9.2876	0.1081	0.1712	0.0434	0.0060
10.00	3.0631	3.3007	9.9727	0.1677	0.0956	0.0288	0.0030
30.00	4.2076	4.3686	11.0407	0.1441	0.0310	0.0152	0.0010
100.00	5.4012	5.4819	12.1539	0.0787	0.0095	0.0078	0.0003

Table XII. Stopping power table for protons in several elements as a function of kinetic energy T. Below 1 MeV, the uncertainty is several percent; above 1 MeV it is mainly determined by the error in the I-value. If a linear interpolation is made for ln S and ln T, the maximum error of interpolated values is 0.1%.

Element:	La	Sm	Er	Ta	Au	Pb	U
Density:	6.189	7.49	9.15	16.6	19.32	11.36	19.07 g/cm ³
I-value:	474	561	650	734	790	779	841 eV

T (MeV)	stopping power (MeV cm ² /g)						
	La	Sm	Er	Ta	Au	Pb	U
0.3	153.79	125.71	106.25	117.29	103.41	103.79	88.36
0.4	136.93	113.95	98.23	101.95	92.02	92.59	82.00
0.5	123.67	105.23	92.06	91.86	84.03	84.52	76.32
0.6	113.16	98.12	86.82	84.52	77.99	78.35	71.54
0.7	104.68	92.15	82.24	78.82	73.18	73.43	67.51
0.8	97.707	87.009	78.179	74.208	69.203	69.360	64.055
0.9	91.875	82.533	74.553	70.333	65.830	65.905	61.071
1.0	86.986	78.624	71.307	67.016	62.910	62.920	58.448
1.2	78.882	72.045	65.735	61.534	58.046	57.961	54.032
1.4	72.543	66.719	61.136	57.174	54.097	53.959	50.433
1.6	67.401	62.304	57.262	53.563	50.820	50.628	47.410
1.8	63.113	58.567	53.949	50.499	48.019	47.798	44.825
2.0	59.470	55.344	51.083	47.861	45.586	45.347	42.571
2.5	52.303	48.957	45.324	42.574	40.677	40.409	38.025
3.0	46.964	44.123	40.965	38.557	36.920	36.641	34.528
3.5	42.793	40.317	37.509	35.374	33.926	33.644	31.736
4.0	39.419	37.222	34.688	32.770	31.470	31.191	29.443
4.5	36.620	34.643	32.334	30.590	29.409	29.135	27.519
5.0	34.254	32.456	30.332	28.734	27.650	27.382	25.875
6.0	30.451	28.927	27.094	25.720	24.791	24.538	23.206
7.0	27.512	26.191	24.575	23.371	22.553	22.316	21.119
8.0	25.160	23.994	22.549	21.475	20.744	20.521	19.435
9.0	23.229	22.185	20.877	19.906	19.249	19.038	18.040
10.0	21.609	20.666	19.470	18.585	17.985	17.787	16.863
12.0	19.038	18.247	17.224	16.470	15.960	15.781	14.978
14.0	17.070	16.393	15.503	14.845	14.400	14.239	13.527
16.0	15.527	14.931	14.135	13.551	13.157	13.009	12.370
18.0	14.266	13.736	13.019	12.494	12.140	12.003	11.422
20.0	13.218	12.742	12.089	11.611	11.289	11.162	10.629
25.0	11.232	10.851	10.317	9.926	9.664	9.555	9.112
30.0	9.823	9.506	9.052	8.719	8.498	8.403	8.023
35.0	8.767	8.495	8.099	7.811	7.618	7.533	7.199
40.0	7.943	7.705	7.354	7.098	6.927	6.851	6.552
50.0	6.737	6.546	6.258	6.048	5.909	5.843	5.595
60.0	5.893	5.732	5.487	5.309	5.190	5.133	4.919
70.0	5.267	5.129	4.913	4.757	4.654	4.603	4.415
80.0	4.783	4.661	4.469	4.330	4.237	4.191	4.022
90.0	4.397	4.288	4.114	3.988	3.904	3.862	3.707
100.0	4.082	3.983	3.823	3.708	3.631	3.592	3.450

Table XIII. Stopping power table for alphas in several elements as a function of kinetic energy T. Below 2 MeV, the uncertainty is several percent; above 1 MeV it is mainly determined by the error in the I-value. If a linear interpolation is made for $\ln S$ and $\ln T$, the maximum error of interpolated values is 0.1%.

Element:	La	Sm	Er	Ta	Au	Pb	U	
A:	138.91	150.35	167.26	180.95	196.97	207.19	238.03	
I-value:	474	561	650	734	790	779	841	eV

T (MeV)	stopping power (MeV cm ² /g)						
	La	Sm	Er	Ta	Au	Pb	U
1.6	557.42	466.11	403.39	417.59	378.14	380.28	337.98
1.8	529.22	447.58	390.41	395.65	360.96	362.94	326.14
2.0	504.17	431.01	378.50	377.19	346.04	347.86	315.03
2.2	481.71	415.85	367.34	361.23	332.94	334.50	304.78
2.4	461.56	401.92	356.82	347.31	321.29	322.61	295.28
2.6	443.45	389.14	347.00	334.94	310.79	311.91	286.51
2.8	426.94	377.24	337.71	323.83	301.32	302.18	278.41
3.0	412.05	366.17	328.92	313.78	292.66	293.32	270.88
3.5	379.91	341.71	309.11	292.28	273.87	274.12	254.28
4.0	354.18	321.03	291.82	274.59	258.22	258.15	240.18
4.5	332.27	303.20	276.65	259.61	244.87	244.54	228.04
5.0	313.65	287.68	263.31	246.71	233.25	232.76	217.42
5.5	297.56	274.03	251.42	235.45	223.03	222.38	208.05
6.0	283.46	261.91	240.77	225.47	213.92	213.14	199.66
7.0	259.86	241.32	222.50	208.47	198.35	197.43	185.27
8.0	240.73	224.35	207.34	194.48	185.41	184.40	173.26
10.0	211.29	198.01	183.51	172.54	164.98	163.87	154.31
12.0	189.43	178.15	165.55	155.95	149.42	148.28	139.81
14.0	172.39	162.56	151.36	142.85	137.08	135.93	128.29
16.0	158.64	149.92	139.81	132.17	126.99	125.85	118.85
18.0	147.26	139.40	130.20	123.25	118.55	117.43	110.96
20.0	137.65	130.50	122.04	115.67	111.35	110.27	104.24
25.0	118.98	113.15	106.08	100.80	97.22	96.22	91.04
30.0	105.34	100.42	94.34	89.82	86.74	85.82	81.27
35.0	94.861	90.606	85.267	81.309	78.627	77.760	73.698
40.0	86.519	82.775	78.010	74.487	72.101	71.304	67.616
50.0	74.003	70.986	67.059	64.164	62.208	61.510	58.407
60.0	65.007	62.456	59.133	56.670	55.009	54.388	51.705
70.0	58.181	56.018	53.088	50.947	49.501	48.944	46.574
80.0	52.806	50.914	48.316	46.412	45.135	44.625	42.501
90.0	48.453	46.772	44.424	42.722	41.575	41.106	39.180
100.0	44.849	43.336	41.211	39.656	38.611	38.176	36.411

Figure captions

FIG. 1. Shell corrections, C_ν , calculated for gold with the nonrelativistic hydrogenic approximation (K-shell: Walske, 1952; L-shells: Bichsel, 1987; M-shells: Bichsel, 1983). The scaled functions ${}_r C_\nu$ are plotted vs. a common, scaled abscissa η . The scaling was chosen to give the ordinate value 1.0 at the maximum for each function and to have the maximum value at the same value of the abscissa, viz. $\eta=0.18$. The actual function, C_ν , can be obtained by using $\eta_\nu = f_\nu \cdot \eta$, and $C_\nu(\eta_\nu) = g_\nu \cdot {}_r C_\nu(\eta)$, where f_ν and g_ν are given below.

			W_ν	f_ν	g_ν	n
K	1s	- - - -	0.876	6.03	1.04	2
LII	2p	-----	0.182	0.999	1.472	2
MI	3s	-.-.-.-.	0.081	0.616	0.561	2
MII	3p	0.072	0.444	1.04	2
MIV	3d	-.-.-.-.	0.039	0.403	3.524	4

The functions for L_I , L_{III} , M_{III} and M_V are not shown (L_I lies very close to M_I). Note that g_ν is not proportional to the number of electrons n in the subshells, and f_ν is only approximately proportional to $W_\nu = J_\nu / \epsilon_\nu$, Eq. (4b).

FIG. 2. Total shell corrections C/Z for protons with kinetic energy T in gold metal. Solid line: present values; dashed-dotted line: calculation by Bonderup (1967), using the Lenz-Jensen model of the atom; dotted line: experimental function used by Andersen and Ziegler (1977); dashed line: Janni (1982). Note that in Eq. (2a) an increased shell correction can give approximately the same L_0 if I is reduced.

FIG. 3. Values of the vertical scaling factor V_3 for the outermost shells, for best fits to different experimental data sets for protons, as a function of atomic number Z for $Z \geq 73$. The parameters $V_1=1.25$, $V_2=1.4$, $H_3=13$ were used for all Z . Resulting I -values differ for each set (Fig. 5). The function $V_3=(Z-46)/25$ is shown as a solid line. It is not possible to assign uncertainties derived from σ_e to individual values because V_3 as well as I would change with changes in S_x . Symbols are related to authors in Table V.

FIG. 4. Same as Fig. 3 for $Z \leq 72$, but data for α with $T \geq 2$ MeV (Er, $Z=68$, Oberlin and Langley) were also included. The following parameters were used: $V_1=1.25$, $V_2=1.4$ for all Z ; $H_3=50$ for $Z < 60$, $H_3=25$ for $Z > 60$ (Table VI). Resulting I -values differ for each set of experimental data. No systematic dependence of V_3 on Z is evident, thus $V_3=3.85$ was chosen as an approximate average for $Z \leq 60$, $V_3=2.3$ for $Z > 60$. For symbols, see Table V.

FIG. 5. Values of the Bloch parameter $b_a = I_a/Z$ for different experimental data sets for protons and α as a function of atomic number Z , with $V_1=1.25$, $V_2=1.4$ for all Z , the other parameters given as a function of Z : for $Z < 60$, $H_3=50$, $V_3=3.85$; for $60 < Z \leq 72$: $H_3=25$, $V_3=2.3$, and for $Z > 72$: $H_3=13$, $V_3=(Z-46)/25$. The different values b_a at each Z express the systematic differences in the experimental data (Table VIa). An uncertainty of $\pm 1\%$ in S_x gives an uncertainty of about $\pm 1\%$ in b_a at 1 MeV, about $\pm 3\%$ at 10 MeV (Table X). The unweighted mean value for $p=18$ measurements in gold is $I=(788 \pm 12)$ eV, for Pb, $p=8$, $I=(779 \pm 25)$ eV.

FIG. 6. Comparison of experimental and theoretical values of the proton and deuteron stopping power for gold. In order to show differences clearly, the relative difference, $r(T)$ (Eq. (11)) is given as a function of the kinetic energy per nucleon, T/M of the particles. The theoretical values were calculated with $V_1=1.25$, $V_2=1.4$, $H_3=13$, $V_3=(Z-46)/25=1.32$, and $I_e=789.9$ eV. Some data are not shown here, but are included in Fig. 6a. Symbols are given in Table V; continuous lines are used for smoothed data: dashed-double dotted: Bader et al. (1956); double-dotted: Green et al. (1955); dashed: Luomajärvi (1979); dashed-dotted: Sørensen and Andersen (1973); solid line above 0.8 MeV: Andersen and Nielsen (1981). The α and Li data by Andersen et al. (1977) between 1 and 4 MeV/M are shown by dotted lines. For the data by Semrad (1990) below 0.8 MeV, a smooth solid line is shown. It differs on the average by less than $\pm 0.7\%$ from S_x , with a maximum difference of $\pm 1.2\%$ (see Fig. 6a). The data by Green et al. and by Bader et al. were not included in the data adjustment of Section III. Thus their deviation is relatively large. Experimental uncertainties, σ_e , given by the authors

are shown for only a few values. Negative values of r imply values of I_x less than I_e .

FIG. 6a. Comparison of experimental and theoretical values of the stopping power for gold for energies per nucleon, T/M , between 0.3 and 3 MeV. Symbols are given in Table V. Individual values of the data by Semrad (1990) are shown. α data by Fontell and Luomajärvi (1979) are shown as the dash-dotted line, those by Matteson et al. (1978) as a solid line between 0.35 and 0.55 MeV/u, for other data see Fig. 6. α data by Lin et al. (1974) differ by less than 1% from those of Fontell and Luomajärvi and are not shown.

For the Luomojärvi and the Andersen-Nielsen data, similar systematic deviations of about $\pm 0.5\%$ of $r(T)$ are seen between 0.8 and 1.5 MeV. There may be a problem in the theory or in the experiments or both in this region. The increase in $r(T)$ for α below $T/M=0.5$ MeV may be due to a reduced charge z^* of the particles.

FIG. 7. Comparison of experimental and theoretical values of the stopping power for tantalum. The relative difference, $r(T)$ in % (Eq. (11)), is given as a function of particle energy per nucleon, T/M . The theoretical values were calculated with $H_3=13$, $V_3=1.08$, and $I_e=734$ eV. Symbols are given in Table V. Experimental error bars are given at only a few values. Continuous lines show data smoothed by the authors. The proton data by Bader et al. (1956) below 0.6 MeV are shown as the dotted line; those of Sørensen and Andersen (1973) above 2.25 MeV as a solid line. The dashed line shows the proton data by Luomajärvi (1979). α -data by Lin et al. (1973) are shown by the solid line ending at 8.5%. For 2 MeV α , $r=(2.9\pm 3)\%$ for Chu et al. (1973).

The difference in r between the Luomojärvi and the Andersen data at neighbouring energies (1.5 and 2.25 MeV) is about 3%, thus equal to the sum of the experimental errors σ_e . I consider it unlikely that this is a problem in the theory.

FIG. 8. Comparison of experimental and theoretical values of the stopping power for lead. The relative difference, $r(T)$, (Eq. (11)) is given as a function of T/M . The theoretical values were calculated with $H_3=13$, $V_3=1.44$, and $I_e=779$ eV.

For individual data points, see symbols in Table V. Values of r for the data by Bader et al. (1956), dashed line, and Green et al. (1955), dotted line, show similar deviation as those for gold. The data by Sørensen and Andersen (1973) are shown by the solid line. The α -data by Borders (1974) for $1.2 \leq T(\text{MeV}) \leq 1.8$ are shown by the solid line.

FIG. 9. Comparison of experimental and theoretical stopping power values for La, Ce and Pr. S_t was calculated with the parameters $H_3=50$, $V_3=3.85$. The I -values $I_e = b_e \cdot Z$ (eV) (Table I) are shown next to the chemical symbol. Symbols are shown in Table V. The solid lines represent the α -data by Knudsen et al. (1980), the dotted line for La those by Lin et al. (1973).

FIG. 10. Comparison of experimental and theoretical stopping power values for Sm, Gd and Dy. S_t is calculated with the parameters $H_3=25$, $V_3=2.3$, and $I_e = b_e \cdot Z$ of Table I. Symbols are defined in Table V. Note that Sirotinin et al. (1984) for Sm and Gd gave two values of S_x at 0.3, 0.4, 0.8 and 1 MeV. Both values are shown. For Gd, the dashed line represents the proton data given by Andersen et al. (1967), the dotted line the α data by Oberlin et al. (1980). The solid lines show the α -data by Knudsen et al. (1980), the dotted line for Dy those by Lin et al. (1973).

FIG. 11. Comparison of experimental and theoretical stopping power values for Ho, Er and Yb. S_t is calculated with the parameters $H_3=25$, $V_3=2.3$, and $I_e = b_e \cdot Z$ of Table I. Symbols are defined in Table V. The solid lines show the α -data by Knudsen et al. (1980). For Er, data by Oberlin et al. (1982) are shown as smoothed lines which were obtained by making a three parameter fit (H_3, V_3, I) to their experimental data; p: dotted line, α : dashed line. The Langley and Blewer (1976) data for Er are shown by the squares: empty for protons, full for α .

FIG. 12. Comparison of experimental and theoretical stopping power values for Hf ($H_3=25$, $V_3=2.3$), W and Ir ($H_3=13$, $V_3=(Z-46)/25$). S_t is calculated with I_e of Table I. For W, the dotted line represents the α -data by Lin et al. (1973), the dashed-dotted line those by Borders (1974), the dashed line the proton data by Luomajarvi (1979), and the solid line those by Chumanov et al. (1979). UCLA data are given for W and Ir

at 20 and 30 MeV. For 2 MeV α , the data by Chu et al.(1973) are plotted as a star at 0.5 MeV.

FIG. 13. Comparison of experimental and theoretical stopping power values for Pt, Bi and U. S_t is calculated with the parameters $H_3=13$, $V_3=(Z-46)/25$ and I_e of Table I. References to the symbols are given in Table V. The proton data for U by Sørensen and Andersen (1973) are shown by the solid line between 2.25 and 18 MeV, as are those for Pt by Andersen et al. (1967). For protons in Bi, the data by Green et al. (1955) are shown by the solid line, those by Knudsen et al. (1980) by the dashed-double dotted line, the α -data by Kuldeep and Jain (1985) are shown by the dotted line, those by Borders (1974) by the dashed line and those by Knudsen et al. (1980) by the dashed-dotted line. For 2 MeV α , the value for Pt by Chu et al.(1973) is plotted as a star at 0.5 MeV/u.

FIG. 14. Comparison between present calculations and some other tabulations. The relative difference r is plotted as a function of proton energy T , for four elements. The solid line represents the function given by Janni (1982), the dashed line that by Andersen and Ziegler (1977), the dotted line that of Williamson et al (1966).

Fig. 1

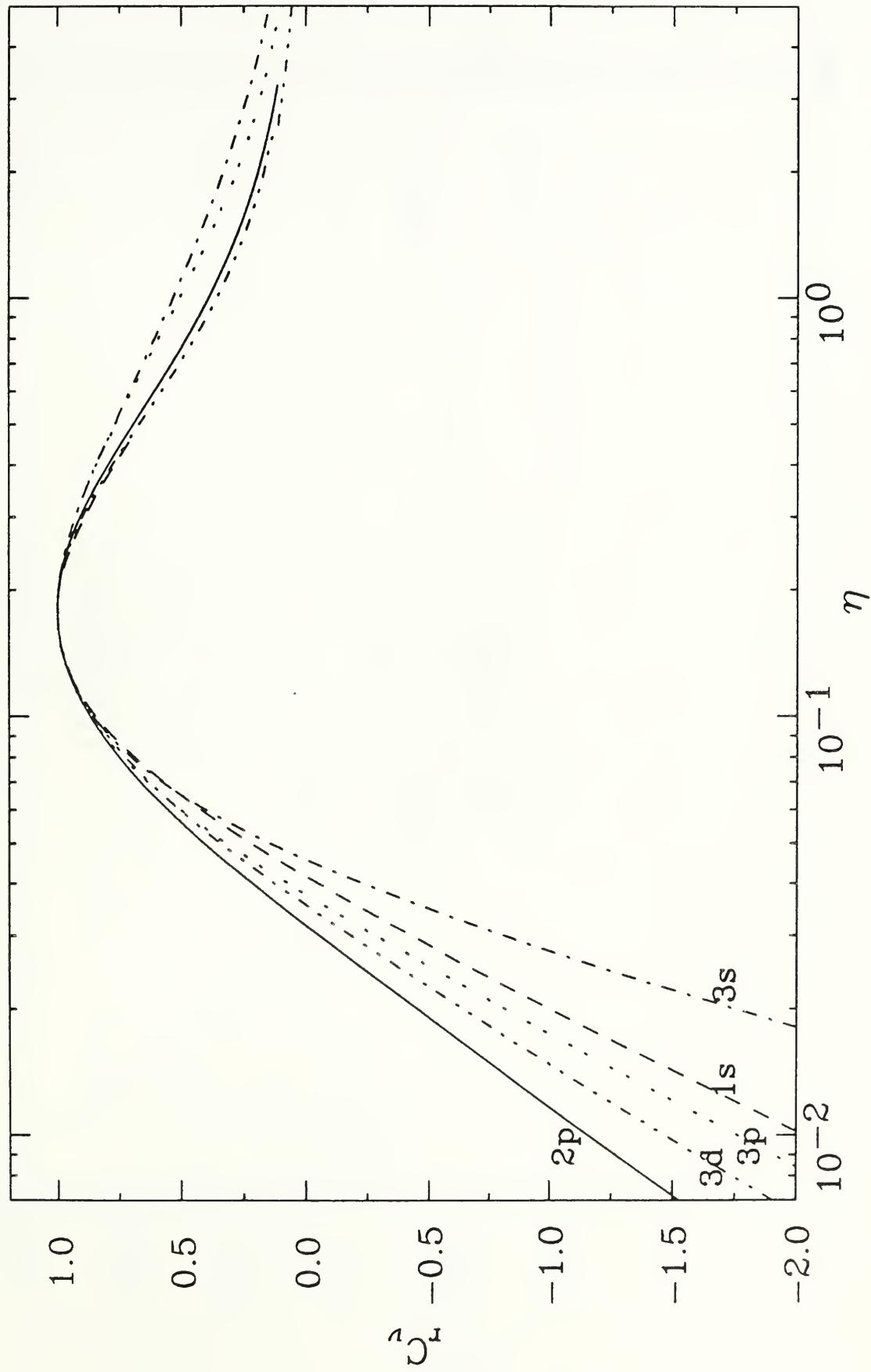


Fig. 2

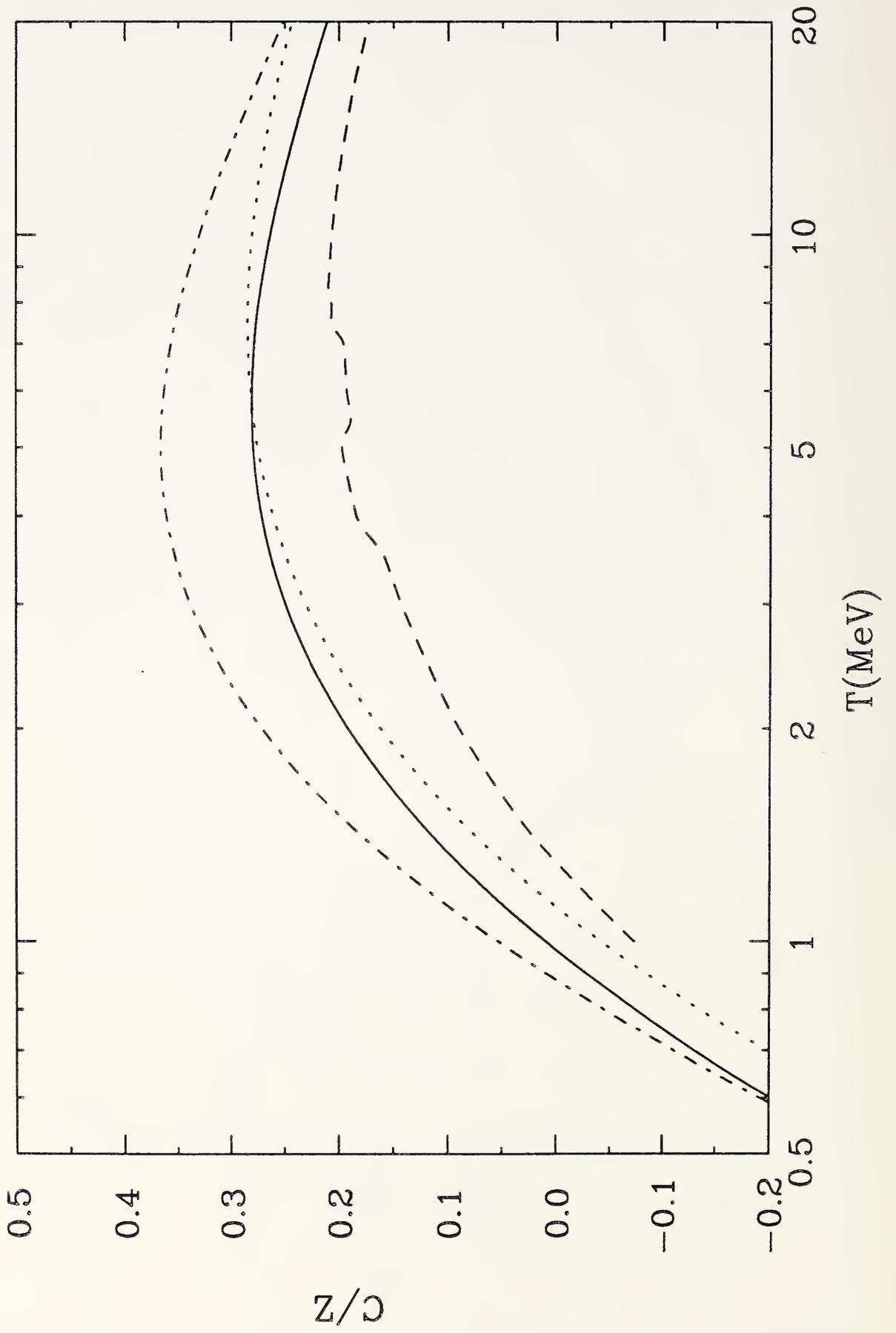


Fig. 4

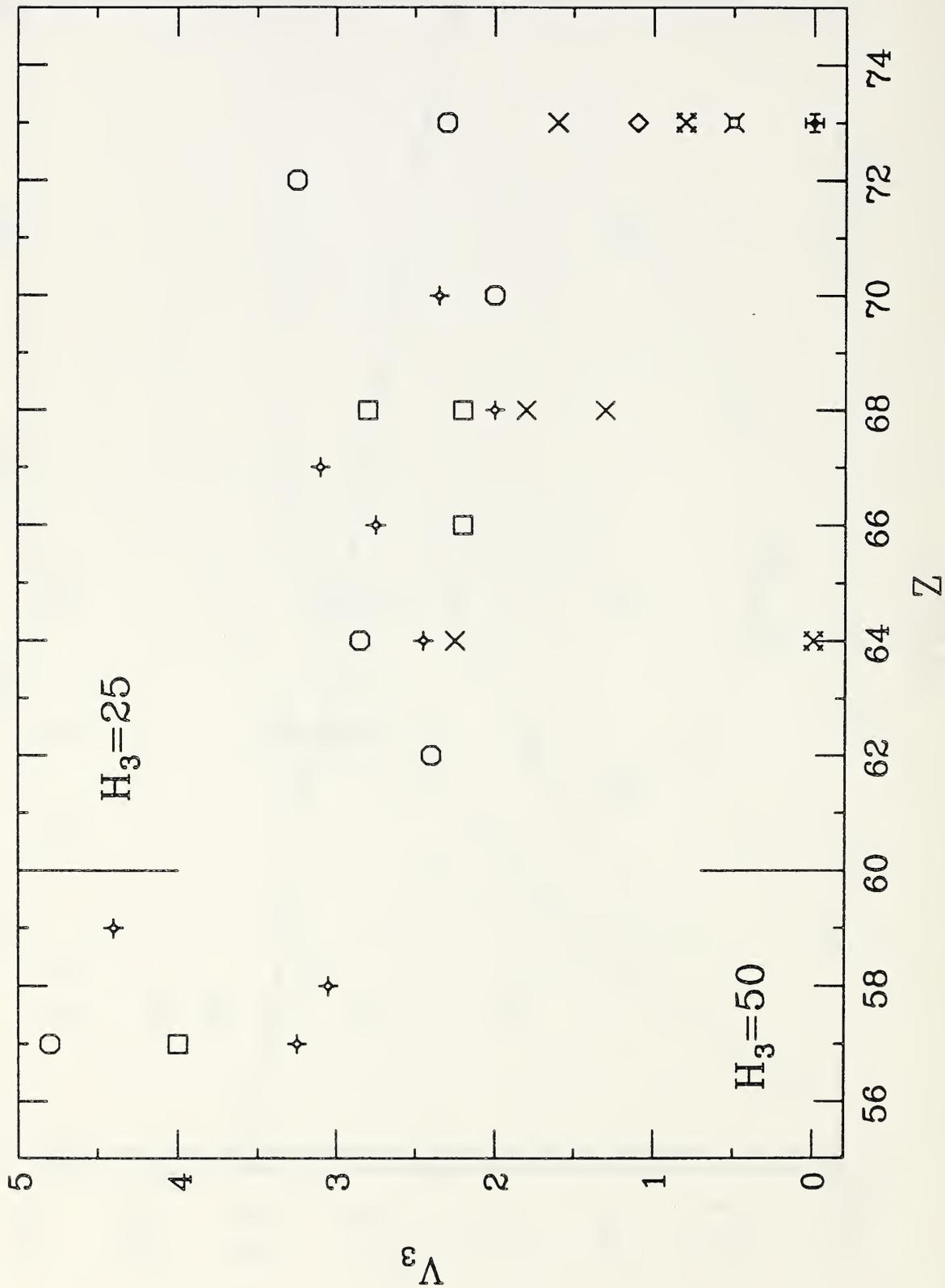


Fig. 5

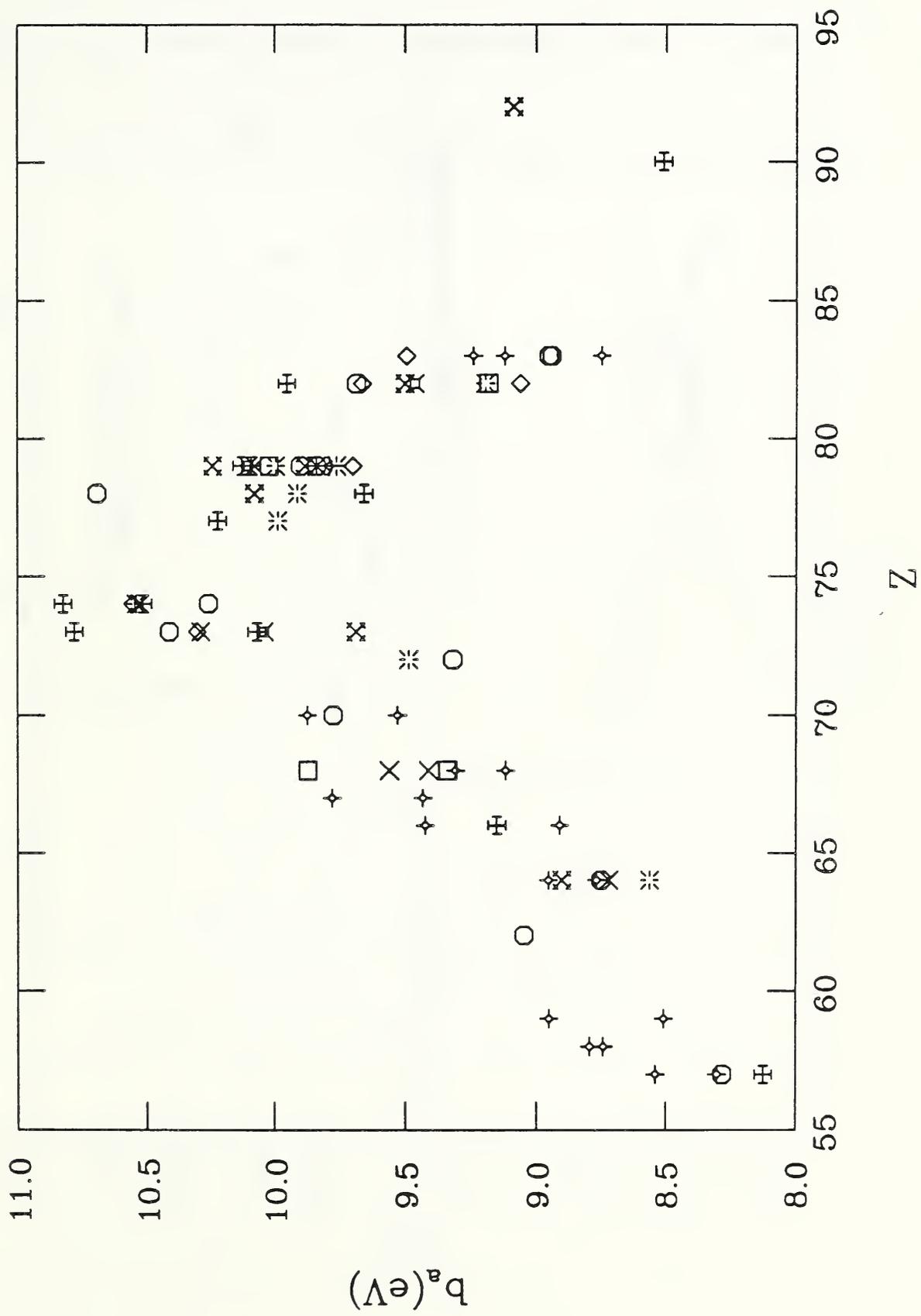


Fig. 6

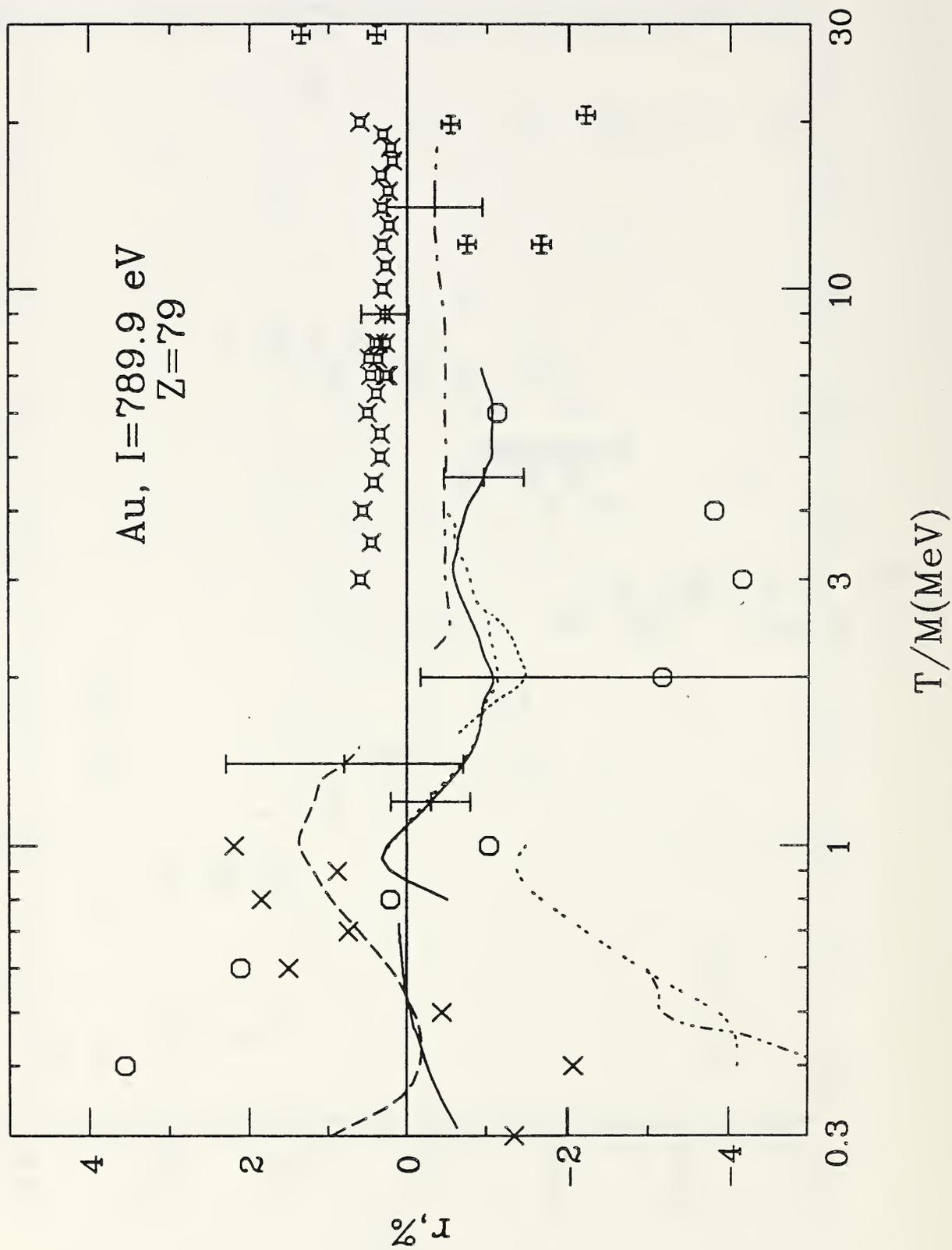


Fig. 7

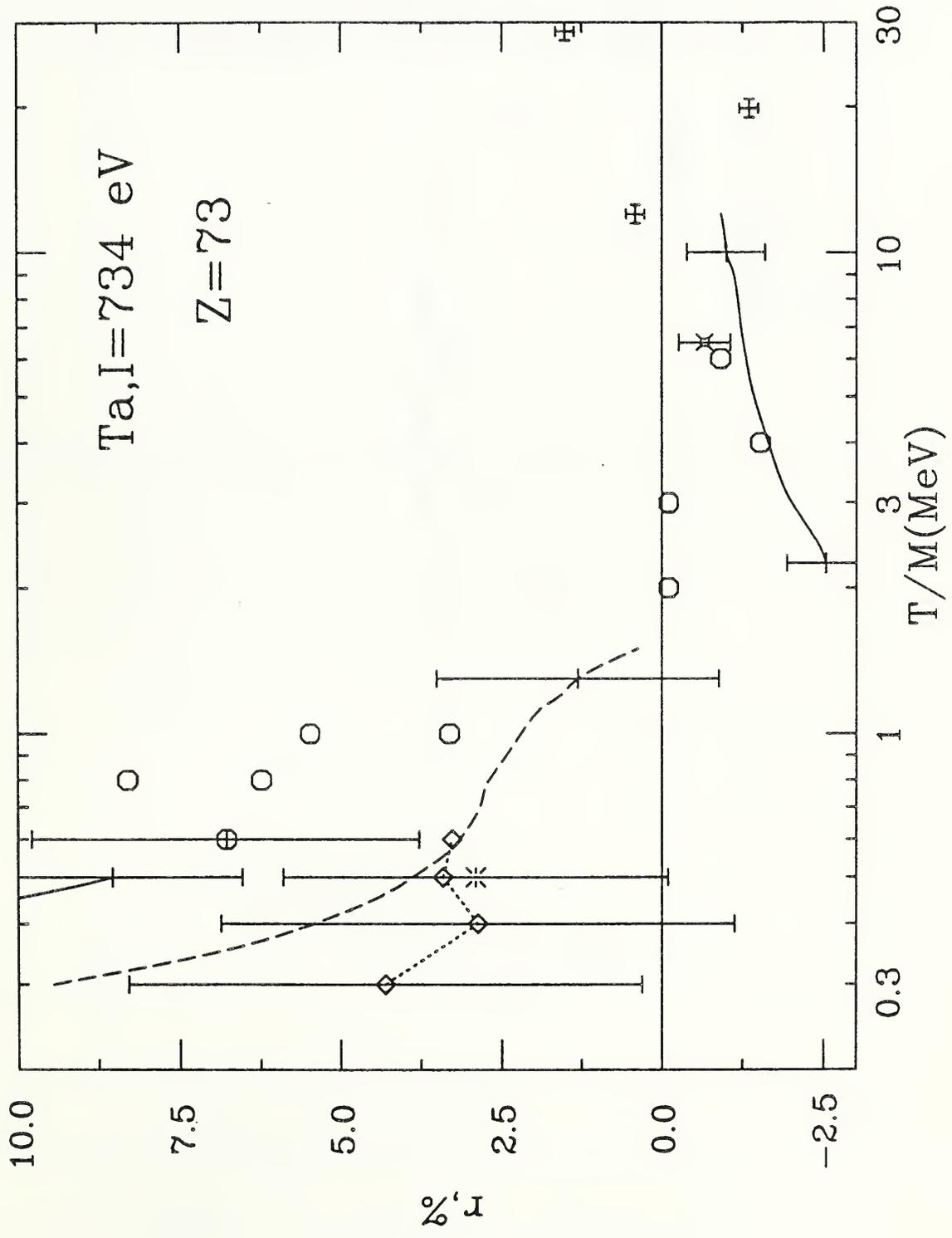


Fig. 8

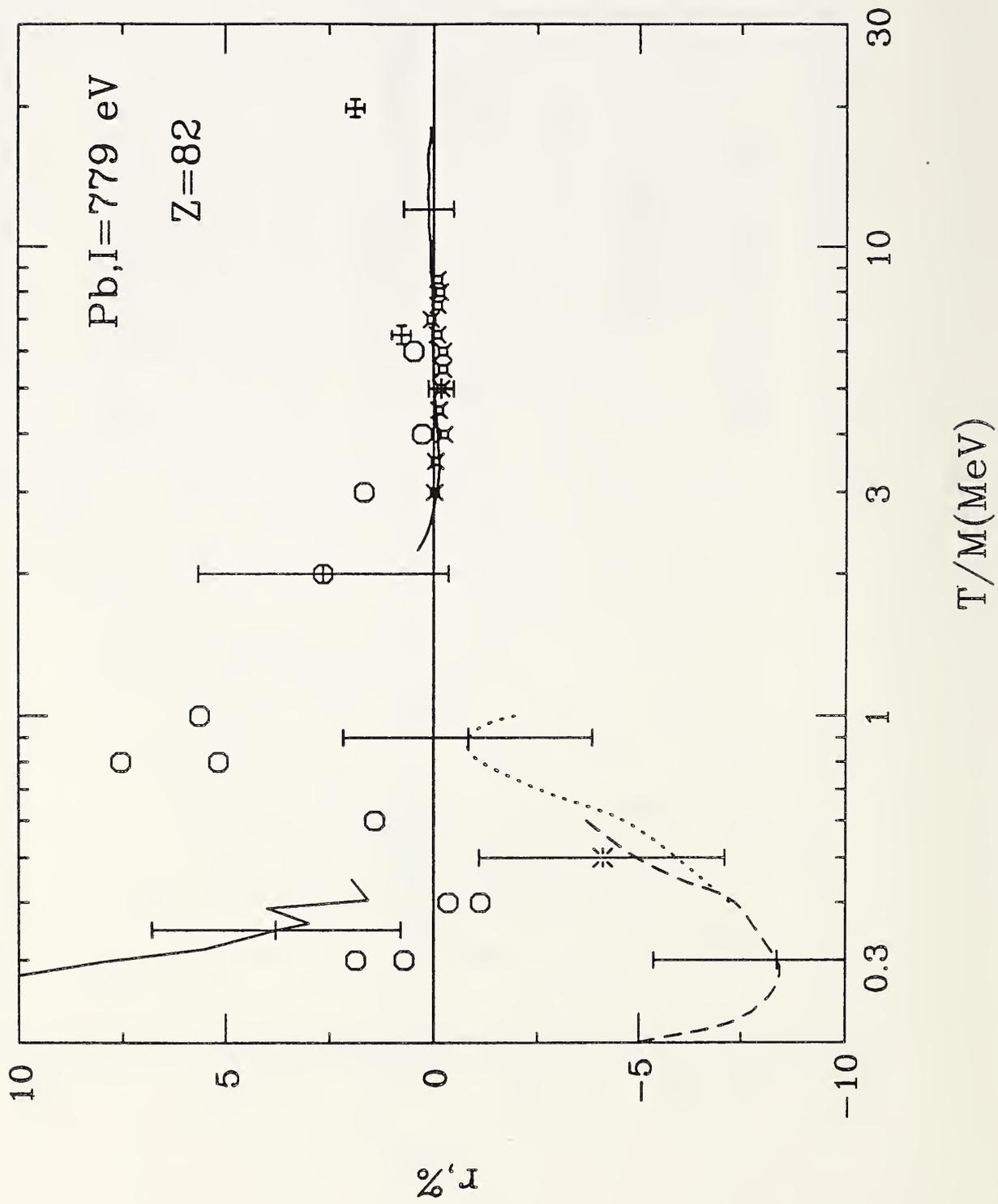


Fig. 9

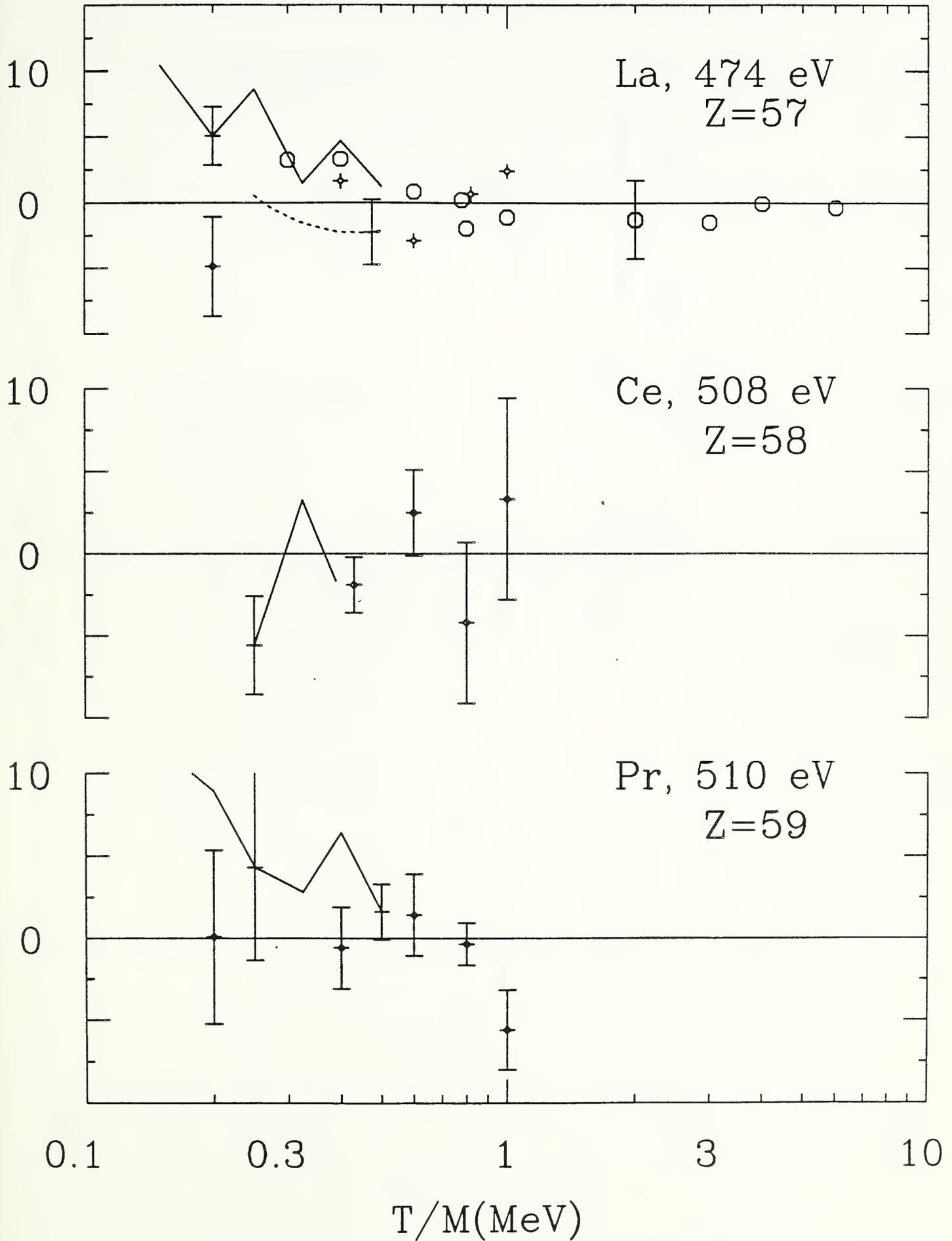


Fig. 10

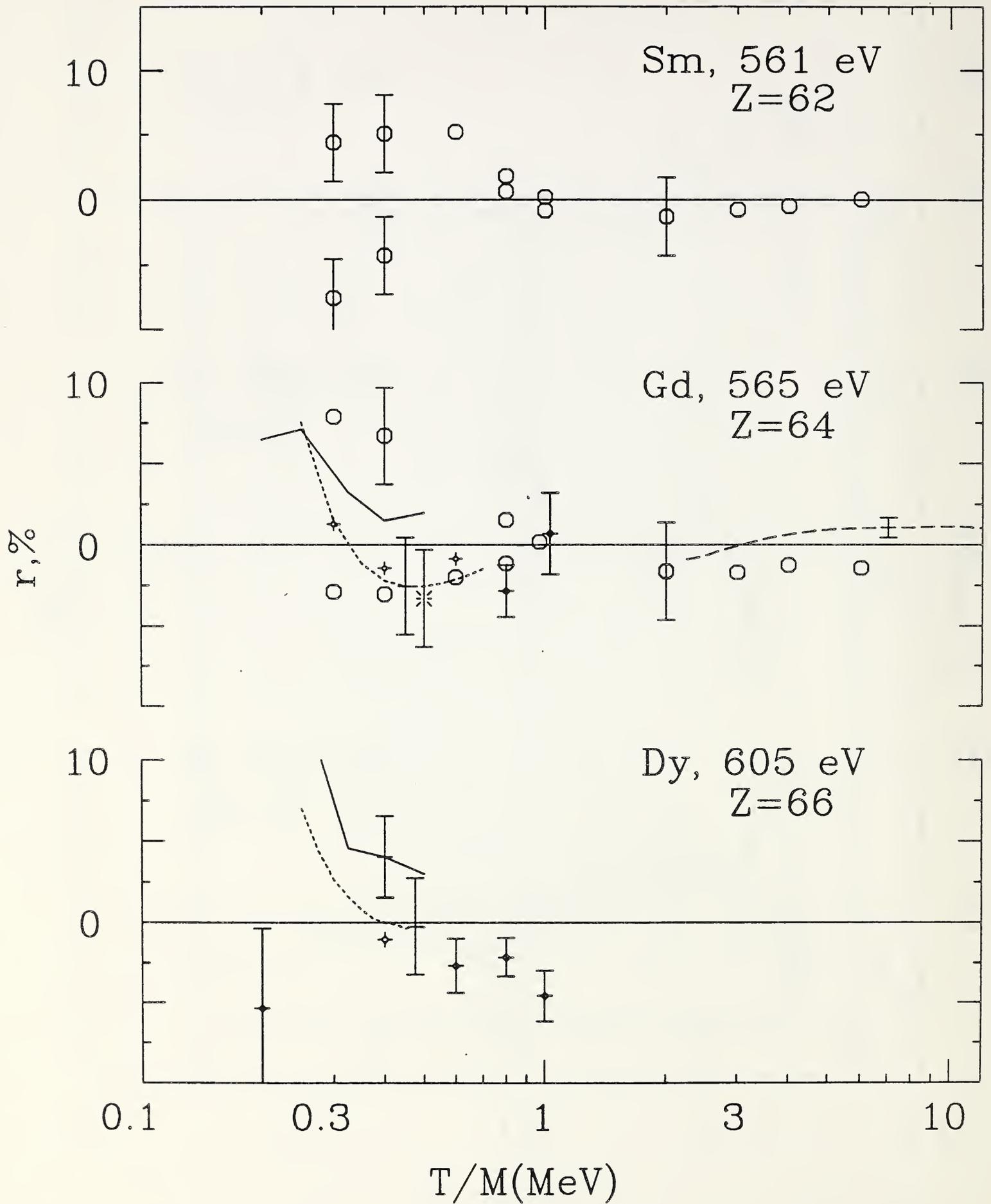


Fig. 11

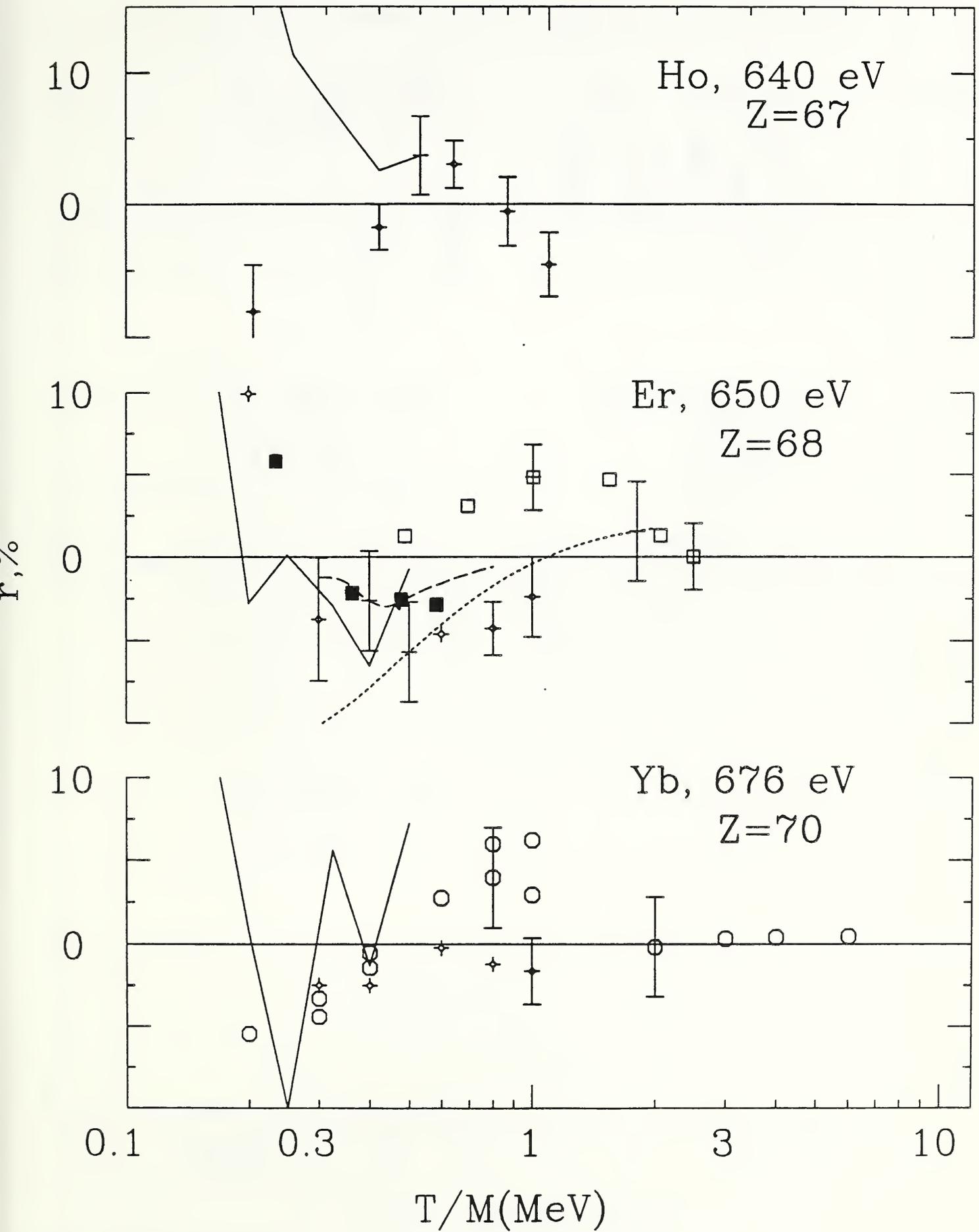


Fig. 12

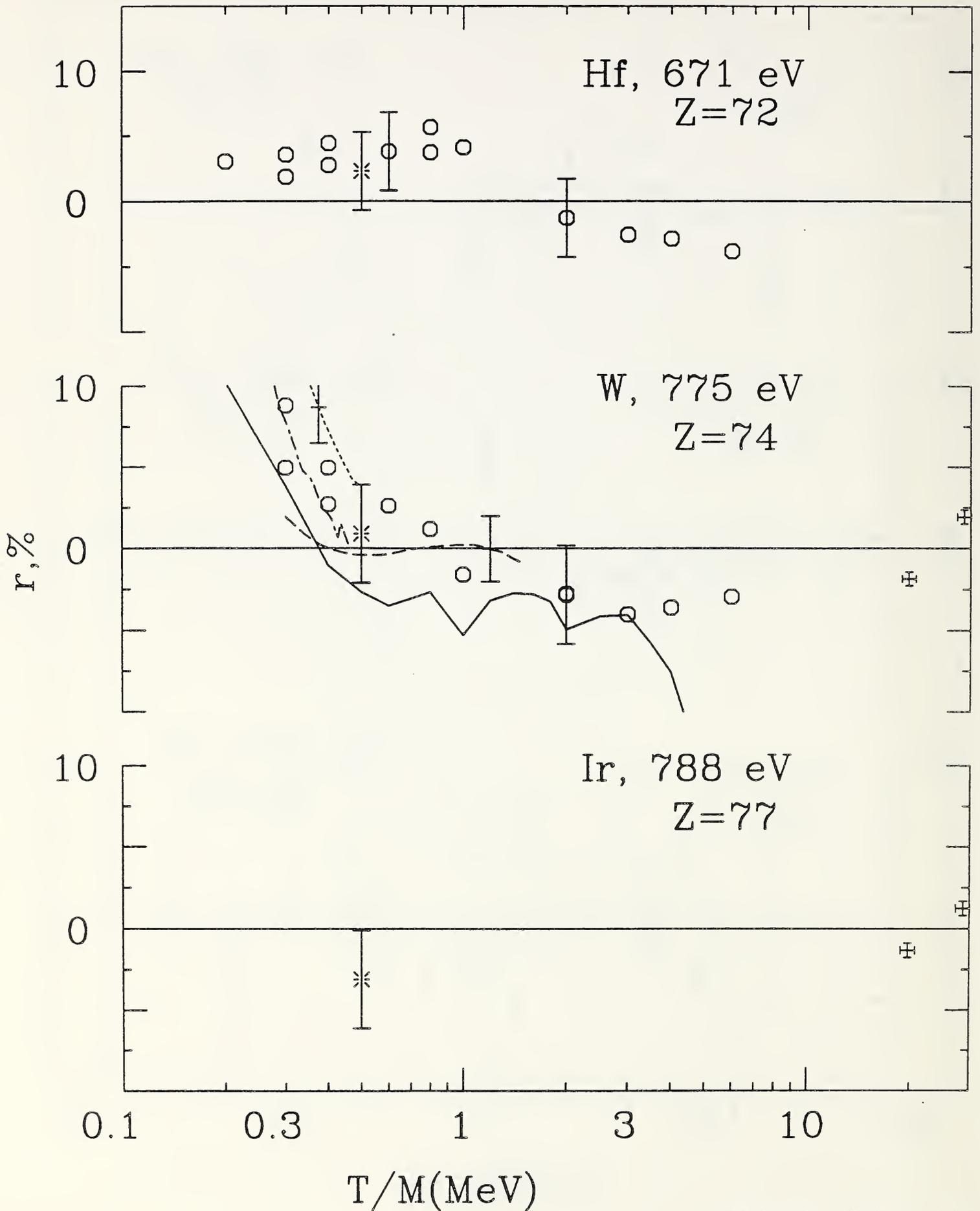


Fig. 13

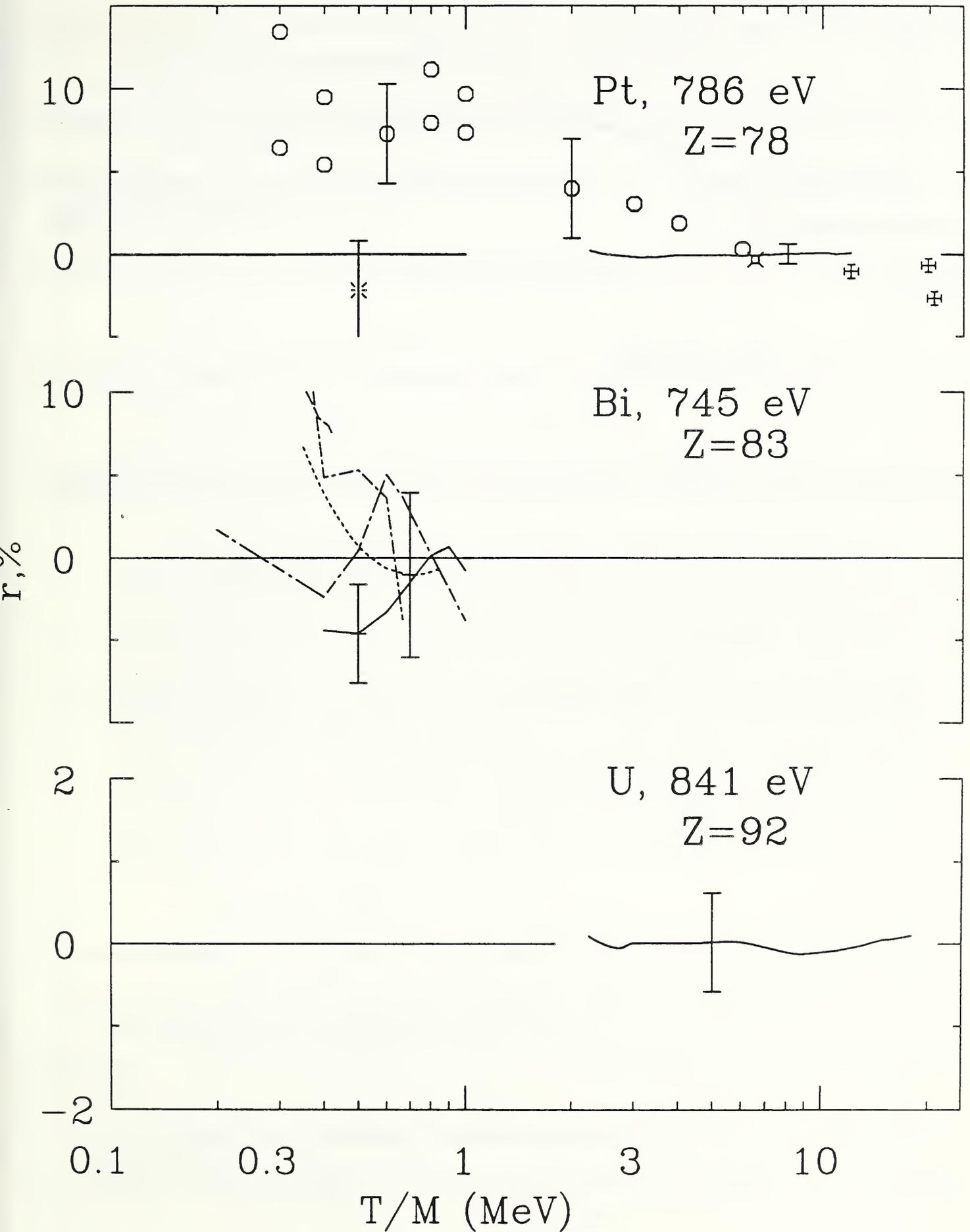
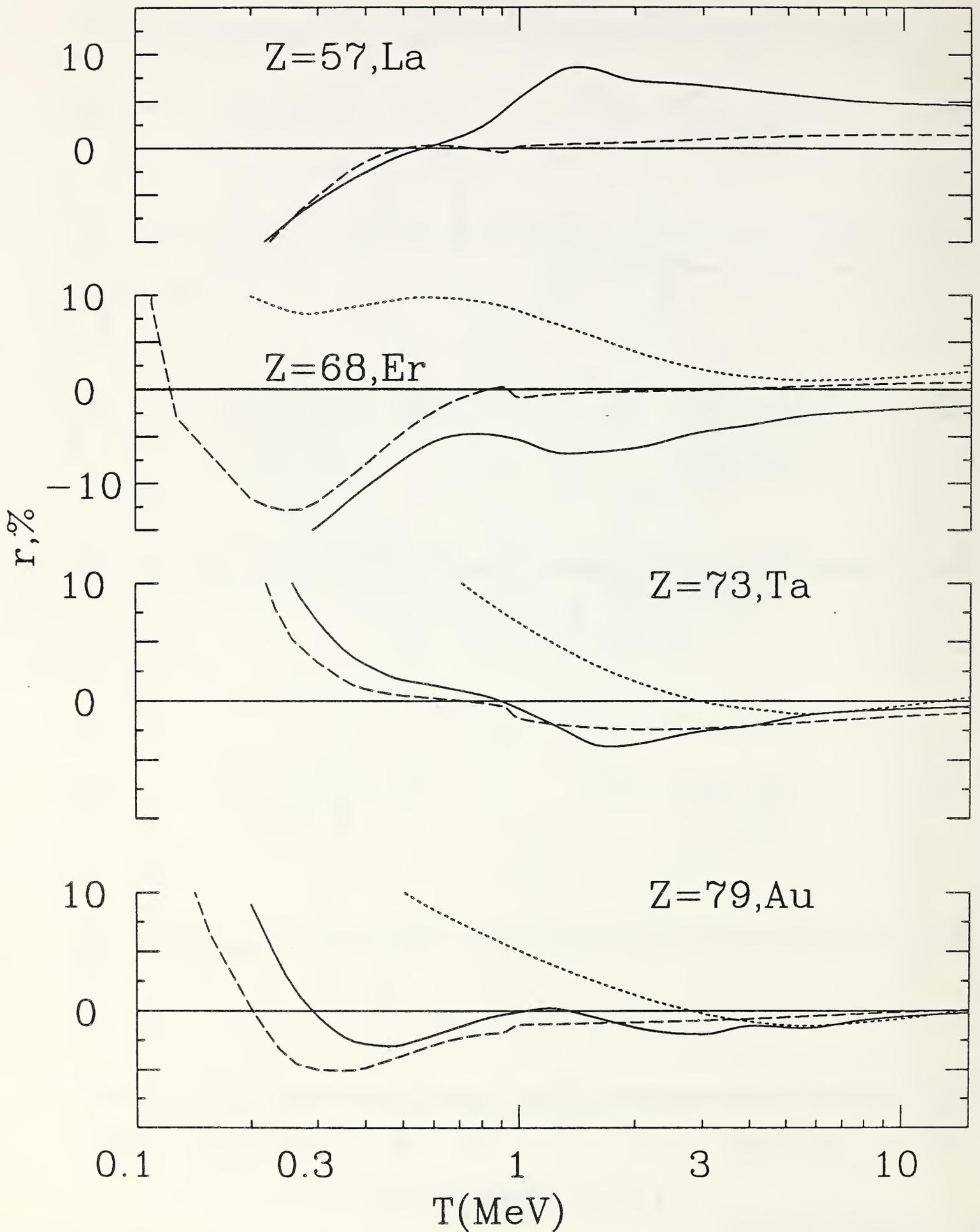


Fig. 14



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11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

The stopping power formula from Bethe's theory contains terms which are known only approximately and must be estimated with the use of experimental data. These terms include a material constant, the mean excitation energy of the medium, and the shell-, Bloch- and Barkas-corrections. In an analysis of measured proton and alpha-particle stopping powers and ranges, modifying parameters have been introduced into these corrections, and the mean excitation energy was simultaneously adjusted, so as to get the closest possible agreement with experimental results. Such an analysis is reported here for elements with atomic numbers $Z \geq 57$. The modification parameters introduced for the shell corrections have a simple relation to atomic energy levels. The Bethe theory with the adopted mean excitation energies and proposed adjustments of the shell- and Barkas-corrections predicts stopping powers that are in close agreement with experimental values, within the experimental uncertainties. This agreement was obtained for protons with kinetic energies above about 0.5 MeV, and for heavier ions of charge z at energies above ($z - 1.5$) MeV/u.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

Bethe theory; charged particles; heavy elements; mean excitation energies; protons; shell corrections; stopping power

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